

## CREATION AND ANNIHILATION OPERATORS

### 6.1 A SIMPLE MATHEMATICAL PROBLEM

In this chapter we shall describe an operator formalism that has widespread applications in quantum mechanics, notably in dealing with harmonic oscillators and in describing many-particle systems.

We begin by formulating and solving the following simple problem: Suppose an operator  $a$  satisfies

$$[a, a^+] = 1. \quad (6.1)$$

The problem is to find the eigenvalues of the Hermitian operator  $a^+a$ , and to relate the eigenvectors. (Note:  $a^+$  denotes the Hermitian conjugate of  $a$ , and  $[A, B]$  is, of course, the commutator  $AB - BA$ .)

We first note that, if  $|\alpha\rangle$  is a normalized eigenvector with

$$a^+a|\alpha\rangle = \alpha|\alpha\rangle, \quad (6.2)$$

then

$$\alpha = \langle\alpha|a^+a|\alpha\rangle = \|a|\alpha\rangle\|^2 \geq 0. \quad (6.3)$$

That is, the eigenvalues are all real and nonnegative. Using the identity  $[AB, C] = A[B, C] + [A, C]B$ , we observe that

$$[a^+a, a] = [a^+, a]a = -a, \quad (6.4)$$

$$[a^+a, a^+] + a^+[a, a^+] = a^+; \quad (6.5)$$

or, equivalently,

$$(a^+a)a = a(a^+a - 1), \quad (6.4')$$

$$(a^+a)a^+ = a^+(a^+a + 1). \quad (6.5')$$

From Eq. (6.4') we have, for an eigenvector  $|\alpha\rangle$ ,

$$(a^+a)a|\alpha\rangle = a(a^+a - 1)|\alpha\rangle = a(\alpha - 1)|\alpha\rangle = (\alpha - 1)a|\alpha\rangle. \quad (6.6)$$

Therefore  $a|\alpha\rangle$  is an eigenvector with eigenvalue  $\alpha - 1$ , unless  $a|\alpha\rangle = 0$ . Similarly  $a^+|\alpha\rangle$  is an eigenvector with eigenvalue  $\alpha + 1$ , unless  $a^+|\alpha\rangle = 0$ . The norm of  $a|\alpha\rangle$  is found from

$$\|a|\alpha\rangle\|^2 = \langle\alpha|a^+a|\alpha\rangle = \alpha\langle\alpha|\alpha\rangle = \alpha,$$

or

$$\|a|\alpha\rangle\| = \sqrt{\alpha}. \quad (6.7)$$

Similarly,

$$\|a^+|\alpha\rangle\| = \sqrt{\alpha + 1}. \quad (6.8)$$

Now, suppose that  $a^n|\alpha\rangle \neq 0$  for all  $n$ . Then by repeated application of Eq. (6.6),  $a^n|\alpha\rangle$  is an eigenvector of  $a^+a$  with eigenvalue  $\alpha - n$ . This contradicts Eq. (6.3), because  $\alpha - n < 0$  for sufficiently large  $n$ . Therefore we must have

$$a^n|\alpha\rangle \neq 0 \quad \text{but} \quad a^{n+1}|\alpha\rangle = 0 \quad (6.9)$$

for some nonnegative integer  $n$ .

Let  $|\alpha - n\rangle = a^n|\alpha\rangle / \|a^n|\alpha\rangle\|$ , so that  $|\alpha - n\rangle$  is a normalized eigenvector with eigenvalue  $\alpha - n$ . Then from Eqs. (6.7) and (6.9),

$$\sqrt{\alpha - n} = \|a|\alpha - n\rangle\| = 0,$$

and therefore  $\alpha = n$ . This shows that the eigenvalues of  $a^+a$  must be nonnegative integers, and that there is a “ground state”  $|0\rangle$  such that

$$a|0\rangle = 0. \quad (6.10)$$

By repeatedly applying  $a^+$  to the ground state we see that  $(a^+)^n|0\rangle$  has the eigenvalue  $n$  and, because of Eq. (6.8), it is never zero. Thus the eigenvalues of  $a^+a$  are 0, 1, 2, 3, . . .

If  $|n\rangle$  is a normalized eigenvector with eigenvalue  $n$ , then, from Eq. (6.8),

$$|n - 1\rangle = (1/\sqrt{n})a|n\rangle$$

is a normalized eigenvector with eigenvalue  $n - 1$ . Also

$$a^+|n - 1\rangle = (1/\sqrt{n})a^+a|n\rangle = \sqrt{n}|n\rangle.$$

So applying  $a^+$  to  $|n - 1\rangle$  gives us back  $|n\rangle$  (within a factor), rather than some other state with eigenvalue  $n$ .

We may then construct the eigenstates of  $a^+a$  as follows: First we find a state  $|0\rangle$  such that

$$a|0\rangle = 0. \quad (6.11)$$

( $|0\rangle$  may be unique; if not, we find other operators commuting with  $a$  and  $a^+$ , and classify the  $|0\rangle$ 's according to their eigenvalues.) Then we define

$$|1\rangle = a^+|0\rangle; \quad |2\rangle = \frac{1}{\sqrt{2}}a^+|1\rangle = \frac{1}{\sqrt{2}}(a^+)^2|0\rangle; \quad \dots$$

and in general

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |0\rangle. \quad (6.12)$$

(Note that we could have included arbitrary phase factors in the definition of  $|n\rangle$ ; our convention here is to make them unity.) With this definition, the  $|n\rangle$  are orthonormal\* and satisfy

$$a^+ |n\rangle = \sqrt{n+1} |n+1\rangle \quad (6.13)$$

$$a |n\rangle = \sqrt{n} |n-1\rangle \quad (6.14)$$

$$a^+ a |n\rangle = n |n\rangle. \quad (6.15)$$

Equations (6.11) through (6.15) form the answer to the problem posed at the beginning of this section.

The operators  $a^+$  and  $a$  are called “raising” and “lowering” operators, respectively, because they raise and lower the eigenvalue of  $a^+ a$ . In later applications  $a^+ a$  will be interpreted as the observable representing the number of particles of a certain kind, in which case  $a^+$  and  $a$  are called “creation” and “annihilation” (destruction operators, or “emission” and “absorption” operators. Equations (6.13) and (6.14) may be alternatively expressed in terms of matrix elements:

$$\langle m | a^+ | n \rangle = \sqrt{n+1} \delta_{m,n+1}, \quad (6.13')$$

$$\langle m | a | n \rangle = \sqrt{n} \delta_{m,n-1}. \quad (6.14')$$

\* For, by (6.12) we have

$$\langle n | m \rangle = \langle 0 | a^n (a^+)^m | 0 \rangle (1/\sqrt{n!m!}).$$

From Eq. (6.1) we easily obtain

$$[a, (a^+)^n] = n(a^+)^{n-1},$$

so that

$$\begin{aligned} \langle 0 | a^n (a^+)^m | 0 \rangle &= \langle 0 | a^{n-1} (a^+)^m a | 0 \rangle + \langle 0 | n a^{n-1} (a^+)^{m-1} | 0 \rangle \\ &= n \langle 0 | a^{n-1} (a^+)^{m-1} | 0 \rangle \\ &= n(n-1) \cdots (n-m+1) \langle 0 | a^{n-m} | 0 \rangle \\ &= n! \delta_{nm} \end{aligned}$$

and the orthonormality follows.

## 6.2 THE LINEAR HARMONIC OSCILLATOR

Our first application of the results of Section 6.1 will be to the one-dimensional harmonic oscillator, which has a Hamiltonian of the form

$$H = \frac{1}{2m} p^2 + \frac{m\omega^2}{2} x^2, \quad (6.16)$$

where  $x$  and  $p$  are the position and momentum operators for the particle and satisfy

$$[x, p] = i\hbar. \quad (6.17)$$

Our task is to find the eigenvalues and eigenstates of  $H$ .

Note that  $\sqrt{(m\omega/\hbar)}x$  and  $(1/\sqrt{m\omega\hbar})p$  are dimensionless. Let us define

$$a = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}} x + i \frac{1}{\sqrt{m\omega\hbar}} p \right). \quad (6.18)$$

Because  $x$  and  $p$  are Hermitian it follows that

$$a^+ = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}} x - i \frac{1}{\sqrt{m\omega\hbar}} p \right). \quad (6.19)$$

From Eq. (6.17) we obtain

$$[a, a^+] = 1. \quad (6.20)$$

Expressing  $x$  and  $p$  in terms of  $a$  and  $a^+$ , we have

$$x = \sqrt{\frac{\hbar}{m\omega}} \frac{a + a^+}{\sqrt{2}}, \quad (6.21)$$

$$p = \sqrt{m\omega\hbar} \frac{a - a^+}{i\sqrt{2}}. \quad (6.22)$$

We get, for the Hamiltonian,

$$H = \frac{\hbar\omega}{2} (a^+ a + a a^+) = \hbar\omega (a^+ a + \frac{1}{2}). \quad (6.23)$$

Thus, the eigenstates of  $H$  are those of  $a^+ a$ . Now we can apply the results of Section 6.1, obtaining the eigenstates  $|0\rangle, |1\rangle, |2\rangle, \dots$  that satisfy

$$H|n\rangle = (n + \frac{1}{2})\hbar\omega|n\rangle. \quad (6.24)$$

The energy levels are thus  $E_n = (n + \frac{1}{2})\hbar\omega$ .

The eigenstates themselves are given by Eqs. (6.11) and (6.12). We can easily obtain the wave functions  $\varphi_n(x) = \langle x|n\rangle$  as follows: from Eqs. (6.18) and (6.11),

$$0 = a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}} \left( x + \frac{i}{m\omega} p \right) |0\rangle. \quad (6.25)$$

Applying  $\langle x|$  and noticing that  $\langle x|p|\varphi\rangle = -i\hbar(d\langle x|\varphi\rangle/dx)$ , we get

$$0 = \sqrt{\frac{m\omega}{2\hbar}} \left( x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) \langle x|0\rangle \quad (6.26)$$

(where  $x$  is now a number, rather than an operator.) Equation (6.26) is merely Eq. (6.11) in coordinate representation, in which it takes the form of a differential equation. Solving it, we get

$$\langle x|0\rangle = A e^{-(m\omega/2\hbar)x^2},$$

where  $A$  is a constant. Normalization requires that

$$\begin{aligned} 1 = \langle 0|0\rangle &= \int_{-\infty}^{\infty} \langle 0|x\rangle \langle x|0\rangle dx = |A|^2 \int_{-\infty}^{\infty} e^{-(m\omega/\hbar)x^2} dx \\ &= |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}}, \end{aligned}$$

so

$$A = e^{i\theta} \left( \frac{m\omega}{\pi\hbar} \right)^{1/4}.$$

The phase  $\theta$  of  $A$  is arbitrary, and we set it equal to zero. Then

$$A = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4},$$

so

$$\langle x|0\rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-(m\omega/2\hbar)x^2}. \quad (6.27)$$

We have thus found the wave function for the ground state. For the other states we apply  $a^+$  according to Eq. (1.12):

$$\langle x|n\rangle = \frac{1}{\sqrt{n!}} \langle x|(a^+)^n|0\rangle. \quad (6.28)$$

Since

$$\begin{aligned}\langle x|a^+ &= \sqrt{\frac{m\omega}{2\hbar}} \langle x| \left( x - \frac{i}{m\omega} p \right) \\ &= \sqrt{\frac{m\omega}{2\hbar}} \left( x - \frac{\hbar}{m\omega} \frac{d}{dx} \right) \langle x|,\end{aligned}$$

we have

$$\begin{aligned}\langle x|n\rangle &= \frac{1}{\sqrt{n!}} \left( \frac{m\omega}{2\hbar} \right)^{n/2} \left( x - \frac{\hbar}{m\omega} \frac{d}{dx} \right)^n \langle x|0\rangle \\ &= \frac{1}{\sqrt{n!}} \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \left( \frac{m\omega}{2\hbar} \right)^{n/2} \left( x - \frac{\hbar}{m\omega} \frac{d}{dx} \right)^n e^{-(m\omega/2\hbar)x^2}.\end{aligned}\quad (6.29)$$

The matrix elements of observables between harmonic oscillator states can be found without having to express the states in coordinate representation and integrating over  $x$ . We simply express the observable in terms of the raising and lowering operators. An example of this procedure is given in the following section.\*

### 6.3 AN ANHARMONIC OSCILLATOR

Suppose a system has the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 + \lambda x^4.\quad (6.30)$$

Assume that  $\lambda$  is small enough ( $\ll \hbar\omega$ ) that we can use first-order perturbation theory, treating  $\lambda x^4$  as a perturbation of the Hamiltonian (Eq. (6.16)). Then the perturbed energy levels are

$$E_n \approx (n + \frac{1}{2})\hbar\omega + \Delta_n,\quad (6.31)$$

where

$$\Delta_n = \langle n|\lambda x^4|n\rangle.\quad (6.32)$$

From Eq. (6.21) we have

$$\Delta_n = \lambda \left( \frac{\hbar}{2m\omega} \right)^2 \langle n|(a + a^+)^4|n\rangle.\quad (6.33)$$

\* *Problem:* Prove that

$$|x\rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left( \frac{m\omega}{2\hbar} x^2 \right) \exp\left[ \left( -\frac{1}{2} \right) \left( a^+ - x \sqrt{\frac{2m\omega}{\hbar}} \right)^2 \right] |0\rangle,$$

where  $f(a^+)$  is interpreted as  $\sum a_n (a^+)^n$ , when  $f(x) = \sum a_n x^n$ . From this formula, find a generating function for  $\langle x|n\rangle$ . (Hint: Prove first that  $[a, f(a^+)] = f'(a^+)$ .)

Expanding  $(a + a^+)^4$  gives us 16 terms, but, thanks to the raising and lowering properties of  $a^+$  and  $a$ , the only terms giving a nonzero expectation value are those with two  $a$ 's and two  $a^+$ 's:

$$\begin{aligned} \langle n|(a + a^+)^4|n\rangle &= \langle n|(a^+a^+aa + a^+aa^+a + a^+aaa^+ \\ &\quad + aa^+a^+a + aa^+aa^+ + aaa^+a^+)|n\rangle \\ &= n(n-1) + n^2 + n(n+1) \\ &\quad + n(n+1) + (n+1)^2 + (n+1)(n+2) \\ &= 6n^2 + 6n + 3, \end{aligned}$$

where we have used Eqs. (6.13) and (6.14) repeatedly. Therefore

$$\Delta_n = 3\lambda \left( \frac{\hbar}{2m\omega} \right)^2 (2n^2 + 2n + 1).$$

#### 6.4 SYSTEMS OF HARMONIC OSCILLATORS

Suppose a system has the Hamiltonian

$$H = \sum_i \frac{1}{2m_i} P_i^2 + \sum_{i,j} V_{ij} Q_i Q_j \quad (6.34)$$

where  $Q_i$  and  $P_i$  are canonical coordinates and momenta:

$$[Q_i, Q_j] = [P_i, P_j] = 0; \quad [Q_i, P_j] = i\hbar\delta_{ij}, \quad (6.35)$$

and  $V_{ij} = V_{ji}$ . To simplify the presentation a little let us make a change of scale, defining

$$q_i = \sqrt{m_i} Q_i; \quad p_i = P_i/\sqrt{m_i} \quad (6.36)$$

and

$$U_{ij} = \frac{2}{\sqrt{m_i m_j}} V_{ij}. \quad (6.37)$$

Then  $q_i$  and  $p_i$  are also canonical:

$$[q_i, p_j] = i\hbar\delta_{ij}, \quad (6.38)$$

and in terms of them the Hamiltonian is

$$H = \frac{1}{2} \sum_i p_i^2 + \frac{1}{2} \sum_{i,j} U_{ij} q_i q_j. \quad (6.39)$$

We shall express  $H$  in terms of raising and lowering operators as we did for the one-dimensional oscillator. The procedure involves two steps: the first is finding a set of normal coordinates  $\tilde{q}_\alpha$  with respect to which the potential is in

diagonal form, and the second is expressing the coordinates and momenta in terms of raising and lowering operators.

Let the coordinates  $q_i$  and  $\tilde{q}_\alpha$  be related by

$$\tilde{q}_\alpha = \sum_i C_{\alpha i} q_i. \quad (6.40)$$

Because  $(U_{ij})$  is assumed to be real and symmetric, the transformation matrix  $C_{\alpha i}$  that diagonalizes it is orthogonal:

$$\sum_i C_{\alpha i} C_{\beta i} = \delta_{\alpha\beta}; \quad \sum_\alpha C_{\alpha i} C_{\alpha j} = \delta_{ij}. \quad (6.41)$$

The inverse transformation of Eq. (6.40) is then

$$q_i = \sum_\alpha C_{i\alpha} \tilde{q}_\alpha. \quad (6.42)$$

We further assume that the eigenvalues of  $(U_{ij})$  are all positive, that is, that the matrix is positive definite (this ensures that  $q_i = 0$  is a point of stable equilibrium). Denoting these eigenvalues by  $\omega_\alpha^2$  ( $\omega_\alpha > 0$ ), we have

$$\sum_{i,j} C_{\alpha i} C_{\beta j} U_{ij} = \omega_\alpha^2 \delta_{\alpha\beta},$$

and thus

$$\sum_{i,j} U_{ij} q_i q_j = \sum_\alpha \omega_\alpha^2 \tilde{q}_\alpha^2. \quad (6.43)$$

Finally, we define  $\tilde{p}_\alpha$  in such a way as to preserve the canonical commutation relations:

$$\tilde{p}_\alpha = \sum_i C_{\alpha i} p_i; \quad (6.44)$$

$$[\tilde{q}_\alpha, \tilde{p}_\beta] = i\hbar \delta_{\alpha\beta}. \quad (6.45)$$

The result of our efforts is that

$$H = \frac{1}{2} \sum_\alpha (\tilde{p}_\alpha^2 + \omega_\alpha^2 \tilde{q}_\alpha^2), \quad (6.46)$$

which means we have a system of decoupled harmonic oscillators (one for each value of  $\alpha$ ).

Using the methods of Section 6.2, we form lowering and raising operators for each mode:

$$a_\alpha = \frac{1}{\sqrt{2\hbar}} \left( \sqrt{\omega_\alpha} \tilde{q}_\alpha + \frac{i}{\sqrt{\omega_\alpha}} \tilde{p}_\alpha \right), \quad (6.47)$$

$$a_\alpha^+ = \frac{1}{\sqrt{2\hbar}} \left( \sqrt{\omega_\alpha} \tilde{q}_\alpha - \frac{i}{\sqrt{\omega_\alpha}} \tilde{p}_\alpha \right), \quad (6.48)$$

$$\tilde{q}_\alpha = \sqrt{\frac{\hbar}{2\omega_\alpha}} (a_\alpha + a_\alpha^\dagger), \quad (6.49)$$

$$\tilde{p}_\alpha = -i \sqrt{\frac{\hbar\omega_\alpha}{2}} (a_\alpha - a_\alpha^\dagger). \quad (6.50)$$

Then,

$$[a_\alpha, a_\beta] = [a_\alpha^\dagger, a_\beta^\dagger] = 0, \quad (6.51)$$

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}, \quad (6.52)$$

$$H = \sum_\alpha \hbar\omega_\alpha (a_\alpha^\dagger a_\alpha + \frac{1}{2}). \quad (6.53)$$

The eigenstates of  $H$  are described by giving, for each  $\alpha$ , the eigenvalue  $n_\alpha$  of  $a_\alpha^\dagger a_\alpha$ . Thus,

$$H|n_1 n_2 n_3 \cdots\rangle = \sum_\alpha (n_\alpha + \frac{1}{2})\hbar\omega_\alpha |n_1 n_2 n_3 \cdots\rangle, \quad (7.54)$$

$$|n_1 n_2 n_3 \cdots\rangle = \left[ \prod_\alpha \frac{(a_\alpha^\dagger)^{n_\alpha}}{\sqrt{n_\alpha!}} \right] |000 \cdots\rangle, \quad (6.55)$$

where the ground state  $|000 \cdots\rangle$  is defined by

$$a_\alpha |000 \cdots\rangle = 0 \text{ for all } \alpha. \quad (6.56)$$

Note that the energy of the ground state is  $\sum_\alpha \frac{1}{2}\hbar\omega_\alpha$ . For a system with infinitely many degrees of freedom (which we will consider shortly), this quantity will generally be infinite. Because the zero point of energy is a matter of definition (only the difference between levels being of physical importance), it is convenient to redefine the Hamiltonian of such a system so that the ground-state energy is zero. Thus, if we let

$$H = \frac{1}{2} \sum_\alpha (p_\alpha^2 + \omega_\alpha^2 q_\alpha^2 - \frac{1}{2}\hbar\omega_\alpha) \quad (6.57)$$

with a corresponding (but more complicated) expression in terms of the original coordinates  $q_i$ , then

$$H = \sum_\alpha \hbar\omega_\alpha a_\alpha^\dagger a_\alpha, \quad (6.58)$$

and

$$H|n_1 n_2 n_3 \cdots\rangle = \sum_\alpha n_\alpha \hbar\omega_\alpha |n_1 n_2 n_3 \cdots\rangle. \quad (6.59)$$

## 6.5 PHONONS

The states of the system considered in the preceding section can be given a simple interpretation in terms of “noninteracting phonons”. Assume that the Hamiltonian is given by Eqs. (6.57) and (6.58), so that the energy of the ground

state is zero. The ground state is then called the “vacuum state” and represents the state of the system in which there are no phonons. If the system is in the state  $|n_1 n_2 n_3 \cdots\rangle$  we say that there are  $n_\alpha$  phonons of type  $\alpha$  ( $\alpha = 1, 2, 3, \dots$ ). The  $n_\alpha$  are called “occupation numbers.” Note that the energy of this state is  $n_1 \hbar \omega_1 + n_2 \hbar \omega_2 + \cdots$ , so that the energy of a single phonon of type  $\alpha$  is  $\hbar \omega_\alpha$ , and the total energy is the sum of the energies of the individual phonons. In other words, the phonons are noninteracting.

Since

$$a_\alpha^+ |n_1 \cdots n_{\alpha-1} n_\alpha n_{\alpha+1} \cdots\rangle = \sqrt{n_\alpha + 1} |n, \dots, n_{\alpha-1}, (n_\alpha + 1), n_{\alpha+1} \cdots\rangle, \quad (6.60)$$

$$a_\alpha |n_1 \cdots n_{\alpha-1} n_\alpha n_{\alpha+1} \cdots\rangle = \sqrt{n_\alpha} |n, \dots, n_{\alpha-1}, (n_\alpha - 1), n_{\alpha+1} \cdots\rangle, \quad (6.61)$$

we may call  $a_\alpha^+$  and  $a_\alpha$  creation and annihilation operators for phonons of type  $\alpha$ . The operator for the number of phonons of type  $\alpha$  is  $a_\alpha^+ a_\alpha$ , and the operator for the total number of phonons is

$$N = \sum_\alpha a_\alpha^+ a_\alpha. \quad (6.62)$$

Let the vacuum state be denoted by  $|0\rangle$ , and let

$$|\alpha\rangle = a_\alpha^+ |0\rangle = |0, \dots, 0, 1, 0, \dots\rangle, \quad (6.63)$$

be the state with  $n_\alpha = 1$  and  $n_{\alpha'} = 0$  for  $\alpha' \neq \alpha$ . A phonon, then, is the system that is described by the states  $|\alpha\rangle$  (i.e., the system whose quantum-mechanical Hilbert space is spanned by the  $|\alpha\rangle$ ). If  $|\alpha\rangle$  and  $|\beta\rangle$  are (one-) phonon states, then

$$\begin{aligned} \langle\alpha|\beta\rangle &= \langle 0|a_\alpha a_\beta^+|0\rangle \\ &= \langle 0|(a_\beta^+ a_\alpha + \delta_{\alpha\beta})|0\rangle \\ &= \delta_{\alpha\beta} \end{aligned} \quad (6.64)$$

so that the states  $|\alpha\rangle$  are orthonormal. To each normal mode of vibration of the original system of harmonic oscillators corresponds a one-phonon state (since they are both indexed by  $\alpha$ ).

We can also use a similar notation for states of two or more phonons, defining

$$|\alpha_1, \dots, \alpha_n\rangle = a_{\alpha_1}^+ \cdots a_{\alpha_n}^+ |0\rangle. \quad (6.65)$$

These states are normalized as they stand if  $\alpha_1, \dots, \alpha_n$  are distinct; otherwise, they have a norm larger than 1. Assume for definiteness that  $\alpha$  takes on the

values 1, 2, 3, . . . . Then the state with  $n_1$ , of the  $\alpha$ 's equal to 1,  $n_2$   $\alpha$ 's equal to 2, and so on, is

$$\begin{aligned} |\underbrace{1, \dots, 1}_{n_1}, \underbrace{2, \dots, 2}_{n_2}, \dots \rangle &= (a_1^+)^{n_1} (a_2^+)^{n_2} \cdots |0\rangle \\ &= \sqrt{n_1! n_2! \cdots} |n_1 n_2 \cdots \rangle \end{aligned} \quad (6.66)$$

so that its norm is  $\sqrt{n_1! n_2! \cdots}$ .

When we deal with only a few phonons at a time, it is usually more convenient to use the notation  $|\alpha_1, \dots, \alpha_n\rangle$  rather than the occupation-number description  $|n_1 n_2 \cdots\rangle$ , especially when  $\alpha$  can take on a continuum of values. The effects of creation and destruction operators on  $|\alpha_1, \dots, \alpha_n\rangle$  are

$$a_\alpha^+ |\alpha_1, \dots, \alpha_n\rangle = |\alpha, \alpha_1, \dots, \alpha_n\rangle \quad (6.67)$$

$$a_\alpha |\alpha_1, \dots, \alpha_n\rangle = \sum_{k=1}^n \delta_{\alpha\alpha_k} |\alpha_1, \dots, \alpha_{k-1}, \alpha_{k+1}, \dots, \alpha_n\rangle \quad (6.68)$$

Equation (6.68) comes from Eq. (6.65) and the relation

$$[a_\alpha, a_{\alpha_1}^+ \cdots a_{\alpha_n}^+] = \sum_{k=1}^n \delta_{\alpha\alpha_k} a_{\alpha_1}^+ \cdots a_{\alpha_{k-1}}^+ a_{\alpha_{k+1}}^+ \cdots a_{\alpha_n}^+.$$

Note that phonons act like Bose particles (insofar as we can call them particles\*), as an arbitrary number of them may be in any given state (i.e.,  $|\alpha, \dots, \alpha\rangle$  exists for any number of  $\alpha$ 's). Their Bose nature is also reflected in the symmetry of the states (e.g.,  $|\alpha, \beta\rangle = |\beta, \alpha\rangle$ ). In Section 6.7 we shall show how the ordinary rules for quantum-mechanically describing systems of many Bose particles lead to a set of states and operators with the same form as those obtained here, so that the interpretation of the oscillator as a system of many Bose particles is correct.

We conclude this section by considering the qualitative effect of an anharmonic perturbation on the oscillator system. Suppose the perturbation has terms of the form

$$\sum_{i,j,k} \Gamma_{ijk} q_i q_j q_k \quad \text{and} \quad \sum_{i,j,k,l} \Gamma_{ijkl} q_i q_j q_k q_l.$$

In terms of creation and annihilation operators, the cubic terms are of the form

$$a_\alpha^+ a_\beta^+ a_\gamma^+, a_\alpha^+ a_\beta^+ a_\gamma, \dots, a_\alpha a_\beta a_\gamma,$$

which always changes the number of phonons (e.g., the first term creates three

\* The phonons will look more like particles (e.g., carrying momentum and energy) when the oscillator system is a field as described in the next section.

new phonons). Thus, if we start with a definite number of phonons and let the Hamiltonian drive the system forward in time,

$$\begin{aligned} |\psi(t)\rangle &= e^{-iHt}|\psi(0)\rangle \\ &= |\psi(0)\rangle - itH|\psi(0)\rangle + O(t^2), \end{aligned}$$

we will soon start finding different numbers of particles. The quartic terms similarly change the number of particles, except for terms like

$$a_\alpha^+ a_\beta^+ a_\gamma a_\delta, a_\alpha^+ a_\beta a_\gamma^+ a_\delta, \dots,$$

which conserve the number of particles but act as a mutual interaction between them; that is, the particles are no longer independent. The description of a mutual interaction will be considered in more detail later.

**Exercise:** Verify that the number-of-phonons operator  $N$ , defined by Eq. (6.62), commutes with a product of creation and destruction operators if and only if the number of  $a^+$ 's equals the number of  $a$ 's in the product.

## 6.6 FIELD QUANTIZATION

A notable example of a system with infinitely many degrees of freedom is a *field*. Examples are the amplitude of sound waves, drumhead vibrations, light, and so on. Consider a real scalar\* field  $\varphi(\mathbf{x})$  whose motion† is described by the Lagrangian‡

$$L(\varphi, \dot{\varphi}) = \frac{1}{2} \int d^3\mathbf{x} \dot{\varphi}(\mathbf{x})\dot{\varphi}(\mathbf{x}) - \frac{1}{2} \int d^3\mathbf{x} \int d^3\mathbf{x}' K(\mathbf{x} - \mathbf{x}')\varphi(\mathbf{x})\varphi(\mathbf{x}'), \quad (6.69)$$

where  $K(\mathbf{x} - \mathbf{x}') = K(\mathbf{x}' - \mathbf{x})$ . The classical equations of motion, found by varying  $\varphi(\mathbf{x})$ , are

$$\begin{aligned} 0 &= \frac{\partial}{\partial t} \frac{\delta L}{\delta \dot{\varphi}(\mathbf{x})} - \frac{\delta L}{\delta \varphi(\mathbf{x})} \\ &= \ddot{\varphi}(\mathbf{x}) + \int d^3\mathbf{x}' K(\mathbf{x} - \mathbf{x}')\varphi(\mathbf{x}'). \end{aligned} \quad (6.70)$$

\* The following procedure can be generalized for a multicomponent field by putting indices on everything.

† Classically  $\varphi(\mathbf{x})$  depends on  $t$ , but (as with  $q_i$  in Section 7.4) we will not show it explicitly. Besides, in the Schrödinger picture, the operator  $\varphi(\mathbf{x})$  is time-independent.

‡ We assume that the system is invariant under translations, so that  $K$  is only a function of  $\mathbf{x} - \mathbf{x}'$ .

Note how Eqs. (6.69) and (6.70) resemble the corresponding equations for the system of harmonic oscillators described in Section 6.4:

$$L = \frac{1}{2} \sum_i \dot{q}_i^2 - \frac{1}{2} \sum_{i,j} U_{ij} q_i q_j,$$

$$0 = \ddot{q}_i + \sum_j U_{ij} q_j.$$

Thus, we are justified in treating the field as a system of harmonic oscillators (at least formally):  $\varphi$  corresponds to the symbol “ $q$ ” and  $\mathbf{x}$  corresponds to  $i$ .  $\varphi(\mathbf{x})$  can be thought of as a separate coordinate of the system for each  $\mathbf{x}$ .

As an example, suppose that

$$K(\mathbf{x} - \mathbf{x}') = -c^2 \nabla^2 \delta^3(\mathbf{x} - \mathbf{x}'). \quad (6.71)$$

Then Eq. (6.69) becomes, after a few integrations by parts,

$$L = \frac{1}{2} \int d^3 \mathbf{x} [\dot{\varphi}(\mathbf{x}) \dot{\varphi}(\mathbf{x}) - c^2 \nabla \varphi(\mathbf{x}) \cdot \nabla \varphi(\mathbf{x})], \quad (6.72)$$

and Eq. (6.70) becomes

$$\nabla^2 \varphi(\mathbf{x}) - \frac{1}{c^2} \ddot{\varphi}(\mathbf{x}) = 0, \quad (6.73)$$

which is the usual wave equation.

If we assume that  $\varphi(\mathbf{x})$  is a coordinate of the system for each  $\mathbf{x}$ , the conjugate momentum to  $\varphi(\mathbf{x})$  is

$$\Pi(\mathbf{x}) = \frac{\delta L}{\delta \dot{\varphi}(\mathbf{x})} = \dot{\varphi}(\mathbf{x}). \quad (6.74)$$

The Hamiltonian is then

$$H = \int d^3 \mathbf{x} \Pi(\mathbf{x}) \dot{\varphi}(\mathbf{x}) - L$$

$$= \frac{1}{2} \int d^3 \mathbf{x} \Pi(\mathbf{x}) \Pi(\mathbf{x}) + \frac{1}{2} \int d^3 \mathbf{x} \int d^3 \mathbf{x}' K(\mathbf{x} - \mathbf{x}') \varphi(\mathbf{x}) \varphi(\mathbf{x}'). \quad (6.75)$$

To quantize the system we let  $\varphi(\mathbf{x})$  and  $\Pi(\mathbf{x})$  be Hermitian operators satisfying

$$[\varphi(\mathbf{x}), \varphi(\mathbf{x}')] = [\Pi(\mathbf{x}), \Pi(\mathbf{x}')] = 0, \quad (6.76)$$

$$[\varphi(\mathbf{x}), \Pi(\mathbf{x}')] = i\hbar \delta^3(\mathbf{x} - \mathbf{x}'), \quad (6.77)$$

and assume that the Hamiltonian is given by Eq. (6.75), except for a scalar term to make the ground-state energy zero.

We next express everything in terms of “normal modes.” The situation turns out to be slightly different from that of Section 6.4 because it is convenient here to use “complex” (that is, non-hermitian) normal coordinates.

Because the system is translationally invariant, we expect that it might help to express the fields in “momentum” representation. Therefore we define

$$\tilde{\varphi}(\mathbf{k}) = \int d^3x \varphi(\mathbf{x}) e^{-i\mathbf{k} \cdot \mathbf{x}} \quad (6.78)$$

$$\tilde{\Pi}(\mathbf{k}) = \int d^3x \Pi(\mathbf{x}) e^{-i\mathbf{k} \cdot \mathbf{x}}. \quad (6.79)$$

The inverse transformation is\*

$$\varphi(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tilde{\varphi}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} \quad (6.80)$$

with a similar expression for  $\Pi(\mathbf{x})$ . Since  $\varphi(\mathbf{x})$  and  $\Pi(\mathbf{x})$  are Hermitian, we have

$$\tilde{\varphi}^+(\mathbf{k}) = \tilde{\varphi}(-\mathbf{k}); \quad \tilde{\Pi}^+(\mathbf{k}) = \tilde{\Pi}(-\mathbf{k}). \quad (6.81)$$

From Eqs. (6.76) and (6.77) we obtain

$$[\tilde{\varphi}(\mathbf{k}), \tilde{\varphi}(\mathbf{k}')] = [\tilde{\Pi}(\mathbf{k}), \tilde{\Pi}(\mathbf{k}')] = 0, \quad (6.82)$$

$$[\tilde{\varphi}(\mathbf{k}), \tilde{\Pi}(\mathbf{k}')] = i\hbar(2\pi)^3 \delta^3(\mathbf{k} + \mathbf{k}'). \quad (6.83)$$

Now let

$$\omega^2(\mathbf{k}) = \int d^3x K(\mathbf{x}) e^{-i\mathbf{k} \cdot \mathbf{x}}. \quad (6.84)$$

From  $K(\mathbf{x}) = K(-\mathbf{x}) = K^*(\mathbf{x})$  it follows that

$$\omega^2(\mathbf{k}) = \omega^2(\mathbf{k})^* = \omega^2(-\mathbf{k}). \quad (6.85)$$

Rewriting the Hamiltonian of Eq. (6.75), we get

$$\begin{aligned} H &= \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} [\tilde{\Pi}(-\mathbf{k})\tilde{\Pi}(\mathbf{k}) + \omega^2(\mathbf{k})\tilde{\varphi}(-\mathbf{k})\tilde{\varphi}(\mathbf{k})] \\ &= \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} [\tilde{\Pi}^+(\mathbf{k})\tilde{\Pi}(\mathbf{k}) + \omega^2(\mathbf{k})\tilde{\varphi}^+(\mathbf{k})\tilde{\varphi}(\mathbf{k})]. \end{aligned} \quad (6.86)$$

We assume that  $\omega^2(\mathbf{k}) > 0$ , so that the Hamiltonian is positive definite. [Thus  $\omega(\mathbf{k})$  is real, and we take  $\omega(\mathbf{k}) > 0$ .]

In the example described in Eqs. (6.71), (6.72), and (6.73),  $\omega(\mathbf{k}) = c|\mathbf{k}|$ .

\* Throughout all of this the following integrals will be useful:

$$\int d^3x e^{-i\mathbf{k} \cdot \mathbf{x}} = (2\pi)^3 \delta^3(\mathbf{k}), \quad \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} = \delta^3(\mathbf{x}).$$

Next we will define annihilation and creation operators (compare Eqs. (6.47) through (6.50)):

$$a(\mathbf{k}) = \frac{1}{\sqrt{2\hbar}} \left[ \sqrt{\omega(\mathbf{k})} \tilde{\varphi}(\mathbf{k}) + \frac{i}{\sqrt{\omega(\mathbf{k})}} \tilde{\Pi}(\mathbf{k}) \right], \quad (6.87)$$

$$a^+(\mathbf{k}) = \frac{1}{\sqrt{2\hbar}} \left[ \sqrt{\omega(\mathbf{k})} \tilde{\varphi}(-\mathbf{k}) - \frac{i}{\sqrt{\omega(\mathbf{k})}} \tilde{\Pi}(-\mathbf{k}) \right], \quad (6.88)$$

or

$$\tilde{\varphi}(\mathbf{k}) = \sqrt{\frac{\hbar}{2\omega(\mathbf{k})}} [a(\mathbf{k}) + a^+(-\mathbf{k})], \quad (6.89)$$

$$\tilde{\Pi}(\mathbf{k}) = -i \sqrt{\frac{\hbar\omega(\mathbf{k})}{2}} [a(\mathbf{k}) - a^+(-\mathbf{k})]. \quad (6.90)$$

The commutation relations are, from Eqs. (6.82) and (6.83),

$$[a(\mathbf{k}), a(\mathbf{k}')] = [a^+(\mathbf{k}), a^+(\mathbf{k}')] = 0, \quad (6.91)$$

$$[a(\mathbf{k}), a^+(\mathbf{k}')] = (2\pi)^3 \delta^3(\mathbf{k} - \mathbf{k}'). \quad (6.92)$$

If we write  $H$  in terms of  $a$  and  $a^+$ , making the change of variable  $\mathbf{k} \rightarrow -\mathbf{k}$  when necessary, we obtain

$$H = \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \hbar\omega(\mathbf{k}) [a^+(\mathbf{k})a(\mathbf{k}) + a(\mathbf{k})a^+(\mathbf{k})]$$

plus a correction term to make the vacuum energy zero. The corrected Hamiltonian is evidently

$$H = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \hbar\omega(\mathbf{k}) a^+(\mathbf{k})a(\mathbf{k}). \quad (6.93)$$

[Note that the correction term is the infinite quantity  $-\frac{1}{2} \int d^3\mathbf{k} \hbar\omega(\mathbf{k}) \delta^3(\mathbf{0})$ . Finally, we express the original field variables in terms of the creation and destruction operators, using Eqs. (6.80), (6.89), and (6.90):

$$\varphi(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sqrt{\frac{\hbar}{2\omega(\mathbf{k})}} [a(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + a^+(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}] \quad (6.94)$$

$$\Pi(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sqrt{\frac{\hbar\omega(\mathbf{k})}{2}} [-ia(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + ia^+(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}]. \quad (6.95)$$

Equations (6.91) through (6.95) are the important results of the quantization procedure.

The commutation relation of Eq. (6.92) may appear strange, in that

$[a(\mathbf{k}), a^+(\mathbf{k})]$  is infinite (instead of unity), so that the analysis of Section 6.1 does not apply directly to  $a(\mathbf{k})$ . Suppose, however, that we use a less singular representation. Choose a complete orthonormal set of functions  $\psi_\alpha(\mathbf{k})$ , where  $\alpha$  is a discrete index:

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3} \psi_\alpha^*(\mathbf{k})\psi_\beta(\mathbf{k}) = \delta_{\alpha\beta}, \quad (6.96)$$

$$\sum_\alpha \psi_\alpha(\mathbf{k})\psi_\alpha^*(\mathbf{k}') = (2\pi)^3\delta^3(\mathbf{k} - \mathbf{k}') \quad (6.97)$$

and define

$$a_\alpha = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \psi_\alpha^*(\mathbf{k})a(\mathbf{k}). \quad (6.98)$$

Then

$$[a_\alpha, a_\beta^+] = \delta_{\alpha\beta}, \quad (6.99)$$

so that we can apply previous results and construct  $|n_1 \cdots n_\alpha \cdots\rangle$ . But these states may not be eigenstates of  $H$ . The states

$$|\mathbf{k}\rangle = a^+(\mathbf{k})|0\rangle, \quad |\mathbf{k}, \mathbf{k}'\rangle = a^+(\mathbf{k})a^+(\mathbf{k}')|0\rangle,$$

and so forth, though unnormalizable, are eigenstates of  $H$ .

What kind of phonons do that unnormalizable states represent? The state  $|\mathbf{k}\rangle$  is a phonon of energy  $\hbar\omega(\mathbf{k})$ , and we may also say that it has momentum  $\hbar\mathbf{k}$ . To discover the reason for this, consider the operator

$$\mathbf{P} = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \hbar\mathbf{k}a^+(\mathbf{k})a(\mathbf{k}), \quad (6.100)$$

which satisfies

$$[\mathbf{P}, a^+(\mathbf{k})] = \hbar\mathbf{k}a^+(\mathbf{k}), \quad [\mathbf{P}, a(\mathbf{k})] = -\hbar\mathbf{k}a(\mathbf{k}) \quad (6.101)$$

so that

$$\mathbf{P}|k_1, k_2, \dots\rangle = (\hbar\mathbf{k} + \hbar\mathbf{k}_2 + \cdots)|k_1, k_2, \dots\rangle. \quad (6.102)$$

Now, from Eqs. (6.94) and (6.101) we obtain

$$[\mathbf{P}, \varphi(\mathbf{x})] = i\hbar\nabla\varphi(\mathbf{x}). \quad (6.103)$$

One can then show that

$$e^{\mathbf{a}\cdot\mathbf{P}/i\hbar}\varphi(\mathbf{x})e^{-\mathbf{a}\cdot\mathbf{P}/i\hbar} = \varphi(\mathbf{x} + \mathbf{a}), \quad (6.104)$$

so that  $\mathbf{P}$  generates translations and is therefore the momentum operator.

In Sections 6.7 and 6.8 we will describe further the relation between the operators and the states they create and destroy, as well as how other operators,

such as the Hamiltonian, can be written in terms of the creation and destruction operators using any basis of states.

*Note:* In relativistic quantum mechanics, when one quantizes a free-particle field with  $\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m^2}$  ( $\hbar = c = 1$ ), a different normalization and summation convention is commonly used for momentum states. Everything is written in terms of  $\int d^3\mathbf{k}/(2\pi)^3 2\omega(\mathbf{k})$  and  $(2\pi)^3 2\omega(\mathbf{k})\delta^3(\mathbf{k} - \mathbf{k}')$ , which happen to be relativistically invariant; to accomplish this change of normalization one uses a “relativistic”  $a(\mathbf{k})$  equal to  $\sqrt{2\omega(\mathbf{k})}$  times our  $a(\mathbf{k})$ . Equations (6.92), (6.93), and (6.94) then become

$$\begin{aligned} [a(\mathbf{k}), a^+(\mathbf{k}')] &= (2\pi)^3 2\omega(\mathbf{k})\delta^3(\mathbf{k} - \mathbf{k}'); \\ H &= \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega(\mathbf{k})} \omega(\mathbf{k}) a^+(\mathbf{k}) a(\mathbf{k}); \\ \varphi(\mathbf{x}) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega(\mathbf{k})} [a(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} + a^+(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}]. \end{aligned}$$

In some texts the  $(2\pi)^3$  is also treated differently. We will not use the relativistic normalization here, but it is mentioned in case the reader finds it elsewhere and wants to reconcile it with our notation.

## 6.7 SYSTEMS OF INDISTINGUISHABLE PARTICLES

In the preceding sections we considered the quantum states of an oscillator system as being states of various numbers of a “particle” called a *phonon*. We identified certain states as one-phonon states, and others as states containing more than one phonon.

In this section we shall follow a different line of reasoning. We will start with a space of states describing a *single* particle, either Bose or Fermi, and construct the multiparticle states according to standard methods. For the Bose case we will arrive at a system of states and operators that is mathematically the same as that found previously for a system of oscillators, thereby showing that the interpretation of oscillator states as many-phonon states is consistent with the usual description of many-particle systems. In the meantime we will have also developed a formalism for dealing with Fermi particles, for which the states do not resemble those of a harmonic-oscillator system.

We will treat the Bose and Fermi cases simultaneously, distinguishing them by the number  $\zeta$ ;

$$\zeta = \begin{cases} +1 & \text{if the particles are Bose} \\ -1 & \text{if the particles are Fermi.} \end{cases} \quad (6.105)$$

We will use the symbol  $\zeta^P$  (where  $P$  is a permutation) to denote 1 for the Bose case and  $(-1)^P$  for the Fermi case.

Consider first the case of distinguishable particles. If  $|\psi_1\rangle, \dots, |\psi_n\rangle$  are one-particle states, then

$$|\psi\rangle = |\psi_1\rangle|\psi_2\rangle\cdots|\psi_n\rangle \quad (6.106)$$

describes the  $n$ -particle state with the  $i$ th particle in state  $|\psi_i\rangle$ . If  $|\varphi\rangle = |\varphi_1\rangle|\varphi_2\rangle\cdots|\varphi_n\rangle$ , then we write

$$\begin{aligned} \langle\varphi|\psi\rangle &= (\langle\varphi_1|\langle\varphi_2|\cdots\langle\varphi_n|)(|\psi_1\rangle|\psi_2\rangle\cdots|\psi_n\rangle) \\ &= \langle\varphi_1|\psi_1\rangle\langle\varphi_2|\psi_2\rangle\cdots\langle\varphi_n|\psi_n\rangle, \end{aligned} \quad (6.107)$$

which defines the inner product  $\langle\varphi|\psi\rangle$ . The Hilbert space describing the  $n$ -particle system is that spanned by all  $n$ th-rank tensors with the form of Eq. (6.106).

The state in which the  $i$ th particle is localized at the point  $\mathbf{x}_i$  is  $|\mathbf{x}_1\rangle|\mathbf{x}_2\rangle\cdots|\mathbf{x}_n\rangle$ . As each  $\mathbf{x}_i$  runs over all space, the resulting states form a complete orthonormal set for the  $n$ -particle space (ignoring spin and other variables):

$$(\langle\mathbf{x}_1|\cdots\langle\mathbf{x}_n|)(|\mathbf{y}_1\rangle\cdots|\mathbf{y}_n\rangle) = \delta^3(\mathbf{x}_1 - \mathbf{y}_1)\cdots\delta^3(\mathbf{x}_n - \mathbf{y}_n), \quad (6.108)$$

$$\int d^3\mathbf{x}_1\cdots\int d^3\mathbf{x}_n(|\mathbf{x}_1\rangle\cdots|\mathbf{x}_n\rangle)(\langle\mathbf{x}_1|\cdots\langle\mathbf{x}_n|) = 1. \quad (6.109)$$

Using this basis we can express the  $n$ -particle states in coordinate representation:

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n) = (\langle\mathbf{x}_1|\cdots\langle\mathbf{x}_n|)\psi\rangle. \quad (6.110)$$

For the particle  $|\psi\rangle$  of Eq. (6.106), we have, using Eq. (6.107),

$$\psi(\mathbf{x}_1, \dots, \mathbf{x}_n) = \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)\cdots\psi_n(\mathbf{x}_n), \quad (6.111)$$

where  $\psi_i(\mathbf{x}_i) = \langle\mathbf{x}_i|\psi_i\rangle$ .

Next, let us consider indistinguishable particles. We assume that the particles obey Bose or Fermi statistics, which means that we must symmetrize or antisymmetrize, respectively, the states obtained in Eq. (6.106). We therefore define

$$|\psi_1\rangle \times |\psi_2\rangle \times \cdots \times |\psi_n\rangle = (1/\sqrt{n!}) \sum_P \zeta^P |\psi_{P(1)}\rangle|\psi_{P(2)}\rangle\cdots|\psi_{P(n)}\rangle, \quad (6.112)$$

where  $P$  runs through all permutations of  $n$  objects. It will often be convenient to write  $|\psi_1, \psi_2, \dots, \psi_n\rangle$  for  $|\psi_1\rangle \times |\psi_2\rangle \times \cdots \times |\psi_n\rangle$ .

The space of  $n$ -particle states is that spanned by all "products" of the form of Eq. (6.112). Note that  $|\psi_1\rangle \times \cdots \times |\psi_n\rangle$  is totally symmetric in the Bose case and totally antisymmetric in the Fermi case, as it should be.

**Example:** Let  $|a\rangle$  and  $|b\rangle$  be two single-particle states. If  $\zeta = +1$  (Bose particles),

$$|a\rangle \times |b\rangle = |a, b\rangle = \frac{1}{\sqrt{2}} (|a\rangle|b\rangle + |b\rangle|a\rangle),$$

$$|a\rangle \times |a\rangle = |a, a\rangle = \sqrt{2}|a\rangle|a\rangle.$$

If  $\zeta = -1$  (Fermi particles)

$$|a, b\rangle = \frac{1}{\sqrt{2}} (|a\rangle|b\rangle - |b\rangle|a\rangle),$$

$$|a, a\rangle = 0.$$

Thus, we have the expected result that two Fermi particles cannot be in the same state.

What is the inner product of two of these  $n$ -particle states? The answer is given by the following theorem\*

$$\langle \varphi_1, \dots, \varphi_n | \psi_1, \dots, \psi_n \rangle = \left| \begin{array}{ccc} \langle \varphi_1 | \psi_1 \rangle & \cdots & \langle \varphi_1 | \psi_n \rangle \\ \langle \varphi_n | \psi_1 \rangle & \cdots & \langle \varphi_n | \psi_n \rangle \end{array} \right|_{\zeta}, \quad (6.113)$$

where, for any  $n \times n$  matrix  $A = (A_{ij})$ ,

$$|A|_{\zeta} \equiv \sum_{\mathbf{P}} \zeta^{\mathbf{P}} A_{1\mathbf{P}(1)} \cdots A_{n\mathbf{P}(n)}. \quad (6.114)$$

That is,  $|A|_{-}$  is the determinant of  $A$ , and  $|A|_{+}$  is what is often called the *permanent* of  $A$ .

*Proof:*

$$\begin{aligned} \langle \varphi_1, \dots, \varphi_n | \psi_1, \dots, \psi_n \rangle &= \frac{1}{n!} \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \zeta^{\mathbf{P}} \zeta^{\mathbf{Q}} (\langle \varphi_{\mathbf{P}(1)} | \cdots \langle \varphi_{\mathbf{P}(n)} |) (| \psi_{\mathbf{Q}(1)} \rangle \cdots | \psi_{\mathbf{Q}(n)} \rangle) \\ &= \frac{1}{n!} \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \zeta^{\mathbf{P}} \zeta^{\mathbf{Q}} \langle \varphi_{\mathbf{P}(1)} | \psi_{\mathbf{Q}(1)} \rangle \cdots \langle \varphi_{\mathbf{P}(n)} | \psi_{\mathbf{Q}(n)} \rangle \\ &= \frac{1}{n!} \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \zeta^{\mathbf{P}} \zeta^{\mathbf{Q}} \langle \varphi_1 | \psi_{\mathbf{Q}^{\mathbf{P}^{-1}(1)}} \rangle \cdots \langle \varphi_n | \psi_{\mathbf{Q}^{\mathbf{P}^{-1}(n)}} \rangle \end{aligned}$$

(where we have permuted the factors by  $\mathbf{P}$ )

$$= \frac{1}{n!} \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \zeta^{\mathbf{Q}^{\mathbf{P}^{-1}}} \langle \varphi_1 | \psi_{\mathbf{Q}^{\mathbf{P}^{-1}(1)}} \rangle \cdots \langle \varphi_n | \psi_{\mathbf{Q}^{\mathbf{P}^{-1}(n)}} \rangle$$

\* Compare this theorem with the well-known formula for vectors in 3-space,

$$(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = \begin{vmatrix} \mathbf{a} \cdot \mathbf{c} & \mathbf{a} \cdot \mathbf{d} \\ \mathbf{b} \cdot \mathbf{c} & \mathbf{b} \cdot \mathbf{d} \end{vmatrix}.$$

(since  $\zeta^P = \zeta^{P^{-1}}$  and  $\zeta^Q \zeta^{P^{-1}} = \zeta^{QP^{-1}}$ )

$$= \frac{1}{n!} \sum_P \sum_R \zeta^R \langle \varphi_1 | \psi_{R(1)} \rangle \cdots \langle \varphi_n | \psi_{R(n)} \rangle$$

(letting  $R = QP^{-1}$ )

$$\begin{aligned} &= \sum_R \zeta^R \langle \varphi_1 | \psi_{R(1)} \rangle \cdots \langle \varphi_n | \psi_{R(n)} \rangle \\ &= |(\langle \varphi_i | \psi_j \rangle)|_{\zeta}, \end{aligned}$$

which is the desired result.

Now let  $\{|1\rangle, |2\rangle, \dots\}$  be a complete orthonormal set of states:

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta}; \quad \sum_{\alpha} |\alpha\rangle \langle \alpha| = 1. \quad (6.115)$$

A complete set of  $n$ -particle states consists of  $|\alpha_1, \alpha_2, \dots, \alpha_n\rangle$ , where  $\alpha_1 \leq \dots \leq \alpha_n$  in the Bose case, and  $\alpha_1 < \dots < \alpha_n$  in the Fermi case. These states are orthogonal to one another, but not always normalized. The reader can show, using Eq. (6.113), that for a complete orthonormal set of states we may take

$$\begin{aligned} &\frac{|\alpha_1, \dots, \alpha_n\rangle}{\sqrt{n_1! n_2! \cdots}} \quad (\alpha_1 \leq \dots \leq \alpha_n) \quad \text{for bosons} \\ &|\alpha_1, \dots, \alpha_n\rangle \quad (\alpha_1 < \dots < \alpha_n) \quad \text{for fermions,} \end{aligned}$$

where  $n_{\alpha}$  is the number of times that  $\alpha$  occurs in the sequence  $\alpha_1, \dots, \alpha_n$  (for Fermi particles,  $n_{\alpha} = 0$  or 1).

For either case the completeness relation can be written in the following convenient form:

$$\frac{1}{n!} \sum_{\alpha_1} \cdots \sum_{\alpha_n} |\alpha_1, \dots, \alpha_n\rangle \langle \alpha_1, \dots, \alpha_n| = 1. \quad (6.116)$$

Here the range of each  $\alpha_i$  is unrestricted, duplication of states being taken care of by the  $1/n!$  and the normalization. In the Fermi case, the terms with non-distinct  $\alpha_i$  are, of course, zero. The 1 on the right-hand side of Eq. (6.116) means the unit operator on the space of (properly symmetrized)  $n$ -particle states. Equation (6.116) can be verified by applying the left side to a state  $|\beta_1, \dots, \beta_n\rangle$  and using Eqs. (6.113) and (6.114).

The case  $n = 0$  may require some explanation. The zero-particle states are tensors of rank zero, that is, scalars (complex numbers). They form a one-dimensional space, all of whose elements are proportional to the number 1. The "state" 1 will be denoted by  $|\text{vac}\rangle$  (or sometimes by  $|0\rangle$ ) and called the "vacuum state." The zero-particle states are thus spanned by the state  $|\text{vac}\rangle$ .

We have constructed, for each  $n$ , a Hilbert space that describes a system of  $n$  particles; thus we have an infinite sequence of spaces. In many processes the number of particles is not constant: particles can be created and destroyed. To describe such processes we need a Hilbert space that contains states of varying numbers of particles. To get such a space we simply combine all the  $n$ -particle spaces into one big space that we may call the *multiparticle space*. A general state in the multiparticle space is of the form

$$|\psi\rangle = |\psi^{(0)}\rangle + |\psi^{(1)}\rangle + |\psi^{(2)}\rangle + |\psi^{(3)}\rangle + \cdots, \quad (6.117)$$

where  $|\psi^{(n)}\rangle$  is an  $n$ -particle state.

We define states of different numbers of particles to be orthogonal to each other, so that if  $|\varphi\rangle$  is another multiparticle state and is expressed in the manner of Eq. (6.117), then

$$\langle\varphi|\psi\rangle \equiv \langle\varphi^{(0)}|\psi^{(0)}\rangle + \langle\varphi^{(1)}|\psi^{(1)}\rangle + \cdots. \quad (6.118)$$

If  $\{|\alpha\rangle\}$  is a complete orthonormal set of states, so that Eq. (6.115) holds, then using Eqs. (6.113), (6.115), and (6.118) we may summarize orthogonality by

$$\langle\alpha_1, \dots, \alpha_n|\beta_1, \dots, \beta_m\rangle = \delta_{nm} \begin{vmatrix} \delta_{\alpha_1\beta_1} & \cdots & \delta_{\alpha_1\beta_n} \\ \delta_{\alpha_n\beta_1} & \cdots & \delta_{\alpha_n\beta_n} \end{vmatrix}. \quad (6.119)$$

From Eq. (6.116) we also have the completeness relation

$$\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\alpha_1, \dots, \alpha_n} |\alpha_1, \dots, \alpha_n\rangle \langle\alpha_1, \dots, \alpha_n| = 1. \quad (6.120)$$

In this equation “1” means the unit operator on the whole multiparticle space.

As an example, suppose we describe the states in coordinate representation. The (unnormalizable) state  $|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle$  describes the situation in which there is one particle each at points  $\mathbf{x}_1, \dots, \mathbf{x}_n$ . Then Eqs. (6.119) and (6.120) become

$$\langle\mathbf{x}_1, \dots, \mathbf{x}_n|\mathbf{y}_1, \dots, \mathbf{y}_m\rangle = \delta_{nm} \begin{vmatrix} \delta^3(\mathbf{x}_1 - \mathbf{y}_1) & \cdots & \delta^3(\mathbf{x}_1 - \mathbf{y}_n) \\ \delta^3(\mathbf{x}_n - \mathbf{y}_1) & \cdots & \delta^3(\mathbf{x}_n - \mathbf{y}_n) \end{vmatrix}, \quad (6.121)$$

$$\sum_{n=0}^{\infty} \frac{1}{n!} \int d^3\mathbf{x}_1 \cdots \int d^3\mathbf{x}_n |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \langle\mathbf{x}_1, \dots, \mathbf{x}_n| = 1 \quad (6.122)$$

We may expand an arbitrary multiparticle state  $|\psi\rangle$  as follows, using Eq. (6.122):

$$|\psi\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^3\mathbf{x}_1 \cdots \int d^3\mathbf{x}_n |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \psi^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n). \quad (6.123)$$

Here

$$\psi^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \langle\mathbf{x}_1, \dots, \mathbf{x}_n|\psi\rangle \quad (6.124)$$

is (if  $|\psi\rangle$  is normalized) the amplitude for the state  $|\psi\rangle$  to have  $n$  particles, one at each  $\mathbf{x}_i$ . Note that  $\psi^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n)$  is symmetric or antisymmetric according to the statistics. Note also that if  $|\psi\rangle$  is an  $n$ -particle state and is of the form  $|\psi_1, \dots, \psi_n\rangle$ , where each  $|\psi_i\rangle$  is a one-particle state, then

$$\psi^{(m)}(\mathbf{x}_1, \dots, \mathbf{x}_n) = 0 \quad \text{unless} \quad m = n;$$

$$\psi^{(n)}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \begin{vmatrix} \psi_1(\mathbf{x}_1) & \cdots & \psi_1(\mathbf{x}_n) \\ \psi_n(\mathbf{x}_1) & \cdots & \psi_n(\mathbf{x}_n) \end{vmatrix}_\zeta, \tag{6.125}$$

where  $\psi_i(\mathbf{x}_j) = \langle \mathbf{x}_j | \psi_i \rangle$ . Equation (6.125) follows from Eqs. (6.124) and (6.113). In the Fermi case the determinant is called the ‘‘Slater determinant.’’

We are now ready to define creation and destruction operators. These operators are fundamental for two reasons; first, we constructed the multi-particle states so that we could describe changing numbers of particles, and we need some operators that can effect this change, and second, other operators, such as the total energy, will turn out to be simply expressible in terms of the creation and destruction operators.

Let  $|\varphi\rangle$  be any one-particle state. We define  $a^+(\varphi)$  to be that linear operator which satisfies

$$a^+(\varphi)|\psi_1, \dots, \psi_n\rangle = |\varphi, \psi_1, \dots, \psi_n\rangle \tag{6.126}$$

for any  $n$ -particle state  $|\psi_1, \dots, \psi_n\rangle$ . For  $n = 0$  this is understood to mean  $a^+(\varphi)|\text{vac}\rangle = |\varphi\rangle$ . We call  $a^+(\varphi)$  the *creation operator* for the state  $|\varphi\rangle$ , and its adjoint  $a(\varphi)$  the *destruction operator*.

A creation operator clearly converts an  $n$ -particle state into an  $(n + 1)$ -particle state. It is easily seen that a destruction operator turns an  $n$ -particle state into an  $(n - 1)$ -particle state and annihilates the vacuum state. To find the effect of  $a(\varphi)$  on an  $n$ -particle state  $|\psi_1 \cdots \psi_n\rangle$  we multiply on the left by an arbitrary  $(n - 1)$ -particle state  $\langle \chi_1 \cdots \chi_{n-1} |$ .

$$\begin{aligned} \langle \chi_1 \cdots \chi_{n-1} | a(\varphi) | \psi_1 \cdots \psi_n \rangle &= \langle \psi_1 \cdots \psi_n | a^+(\varphi) | \chi_1 \cdots \chi_{n-1} \rangle^* \\ &= \langle \psi_1 \cdots \psi_n | \varphi, \chi_1 \cdots \chi_{n-1} \rangle^* \\ &= \begin{vmatrix} \langle \psi_1 | \varphi \rangle \langle \psi_1 | \chi_1 \rangle & \cdots & \langle \psi_1 | \chi_{n-1} \rangle \\ \langle \psi_n | \varphi \rangle \langle \psi_n | \chi_1 \rangle & \cdots & \langle \psi_n | \chi_{n-1} \rangle \end{vmatrix}_\zeta^* \\ &= \left\{ \sum_{k=1}^n \zeta^{k-1} \langle \psi_k | \varphi \rangle \begin{vmatrix} \langle \psi_1 | \chi_1 \rangle & \cdots & \langle \psi_1 | \chi_{n-1} \rangle \\ \langle \psi_n | \chi_1 \rangle & \cdots & \langle \psi_n | \chi_{n-1} \rangle \end{vmatrix}_\zeta \right\}^* \end{aligned}$$

(an expansion by minors)

$$\begin{aligned} &= \sum_{k=1}^n \zeta^{k-1} \langle \psi_k | \varphi \rangle^* \langle \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n | \chi_1 \cdots \chi_{n-1} \rangle^* \\ &= \sum_{k=1}^n \zeta^{k-1} \langle \varphi | \psi_k \rangle \langle \chi_1 \cdots \chi_{n-1} | \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n \rangle. \end{aligned}$$

Because this is for arbitrary  $\langle \chi_1 \cdots \chi_{n-1} |$  we have finally,

$$a(\varphi) | \psi_1 \cdots \psi_n \rangle = \sum_{k=1}^n \zeta^{k-1} \langle \varphi | \psi_k \rangle | \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n \rangle. \quad (6.127)$$

Thus the destruction operator removes the states  $|\psi_i\rangle$ , one at a time, leaving a sum of  $(n - 1)$ -particle states. In the Bose case ( $\zeta = 1$ ) the terms all have a + sign, whereas in the Fermi case ( $\zeta = -1$ ) they alternate in sign.

Equations (6.126) and (6.127) describe the action of creation and destruction operators on many-particle states. From Eq. (6.126) it follows that

$$a^+(\varphi_1)a^+(\varphi_2) = \zeta a^+(\varphi_2)a^+(\varphi_1),$$

or

$$[a^+(\varphi_1), a^+(\varphi_2)]_{-\zeta} = 0, \quad (6.128)$$

where  $[A, B]_{-\zeta} \equiv AB - \zeta BA$ ; that is,  $[AB]_{-\zeta}$  ( $\zeta = +1$ ) is the commutator and  $[A, B]_{+\zeta}$  ( $\zeta = -1$ ) is the anticommutator.

Taking the adjoint of Eq. (6.128) we obtain the further result

$$[a(\varphi_1), a(\varphi_2)]_{-\zeta} = 0. \quad (6.129)$$

Thus, the creation operators commute for Bose particles and anticommute for Fermi particles, and similarly for destruction operators.

Now, what is  $[a(\varphi_1), a^+(\varphi_2)]_{-\zeta}$ ? Does it (or any similar expression) reduce to anything simple? We first calculate

$$\begin{aligned} &a(\varphi_1)a^+(\varphi_2)|\psi_1 \cdots \psi_n\rangle \\ &= a(\varphi_1)|(\varphi_2, \psi_1 \cdots \psi_n\rangle \\ &= \langle \varphi_1 | \varphi_2 \rangle |\psi_1 \cdots \psi_n\rangle + \sum_{k=1}^n \zeta^k \langle \varphi_1 | \psi_k \rangle | \varphi_2, \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n \rangle, \end{aligned} \quad (6.130)$$

and then

$$\begin{aligned} a^+(\varphi_2)a(\varphi_1)|\psi_1 \cdots \psi_n\rangle &= \sum_{k=1}^n \zeta^{k-1} \langle \varphi_1 | \psi_k \rangle a^+(\varphi_2)|\psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n\rangle \\ &= \sum_{k=1}^n \zeta^{k-1} \langle \varphi_1 | \psi_k, | \varphi_2, \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_n \rangle. \end{aligned} \quad (6.131)$$

Multiplying Eq. (6.131) by  $\zeta$  and subtracting it from Eq. (6.130) we see that

$$[a(\varphi_1), a^+(\varphi_2)]_{-\zeta} = \langle \varphi_1 | \varphi_2 \rangle. \quad (6.132)$$

Equations (6.128), (6.129), and (6.132) are the fundamental “commutation” relations for creation and destruction operators.

The relations we have derived are usually stated in terms of an orthonormal basis, and we shall now do that. Let  $\{|\alpha\rangle\} = \{|1\rangle, |2\rangle, \dots\}$  be a complete orthonormal set of one-particle states. It is usual to let  $a_\alpha = a(\alpha)$ . Then, since  $\langle \alpha | \beta \rangle = \delta_{\alpha\beta}$ , we have  $[a_\alpha, a_\beta^+]_{-\zeta} = \delta_{\alpha\beta}$ . We consider the Bose and Fermi cases separately.

### Bose Case

Let

$$|n_1 n_2 \dots\rangle = \frac{|1, \dots, 1, 2, \dots, 2, \dots\rangle}{\sqrt{n_1! n_2! \dots}}, \quad (6.133)$$

where  $n_\alpha$  is the number of times  $\alpha$  appears in the ket on the right. Then the  $|n_1 n_2 \dots\rangle$  (each  $n_\alpha = 0, 1, 2, 3, \dots$ ) form an orthonormal basis for the whole multiparticle space. From Eqs. (6.133), (6.126), and (6.127) we find

$$a_\alpha^+ |n_1 n_2 \dots n_\alpha \dots\rangle = \sqrt{n_\alpha + 1} |n_1 n_2 \dots n_\alpha + 1 \dots\rangle, \quad (6.134)$$

$$a_\alpha |n_1 n_2 \dots n_\alpha \dots\rangle = \sqrt{n_\alpha} |n_1 n_2 \dots n_{\alpha-1} \dots\rangle. \quad (6.135)$$

The commutation relations are

$$[a_\alpha, a_\beta] = [a_\alpha^+, a_\beta^+] = 0; \quad [a_\alpha, a_\beta^+] = \delta_{\alpha\beta}. \quad (6.136)$$

Equations (6.134), (6.135), and (6.136) are identical to Eqs. (6.60), (6.61), (6.51), and (6.52) for raising and lowering operators for a system of harmonic oscillators. The operator for the number of particles in the state  $|\alpha\rangle$  is

$$N_\alpha = a_\alpha^+ a_\alpha.$$

The notation of Eq. (6.133) (in terms of “occupation numbers”) is generally not the most convenient. It is more natural, in fact, to continue using the notation we have been using all along in this section, that is, the notation  $|\alpha_1, \alpha_2, \dots, \alpha_n\rangle$ . This notation was discussed in Section 6.5 in connection with phonons. Note that Eqs. (6.126) and (6.127) of this section, when applied to states of the form  $|\alpha_1, \dots, \alpha_n\rangle$ , become identical to Eqs. (6.67) and (6.68). Thus, creation and destruction operators for a system of Bose particles look just like those for what we called a “phonon” system.

### Fermi Case

Using the notation  $|\alpha_1, \dots, \alpha_n\rangle$ , we have

$$a_\alpha^+ |\alpha_1, \dots, \alpha_n\rangle = |\alpha, \alpha_1, \dots, \alpha_n\rangle \quad (6.137)$$

and

$$a_\alpha |\alpha_1, \dots, \alpha_n\rangle = \sum_{k=1}^n (-1)^{k-1} \delta_{\alpha\alpha_k} |\alpha_1, \dots, \alpha_{k-1}, \alpha_{k+1}, \dots, \alpha_n\rangle \quad (6.138)$$

We could also use the occupation-number notation

$$|n_1 n_2 \dots\rangle = |\alpha_1, \alpha_2 \dots\rangle$$

where  $\alpha_1 < \alpha_2 < \dots$ , and  $n_\alpha$  is the number of times  $\alpha$  occurs ( $n_\alpha = 0$  or  $1$ ) in this sequence. If  $n_\alpha = 0$ , then  $a_\alpha^+$  changes it to  $1$ , whereas  $a_\alpha$  annihilates the state. If  $n_\alpha = 1$ , then  $a_\alpha$  changes it to  $0$ , whereas  $a_\alpha^+$  annihilates the state. There are also factors of  $\pm 1$  involved, depending on what other states are occupied. It is easiest merely to remember Eqs. (6.137) and (6.138).

Note that  $a(\varphi)^2 = a^+(\varphi)^2 = 0$  for any one-particle state  $|\varphi\rangle$ . This statement follows from Eqs. (6.128) and (6.129) (with  $\zeta = -1$  and  $\varphi_1 = \varphi_2 = \varphi$ ), and it is also equivalent to the fact that two fermions cannot be in the same state, that is,  $|\varphi, \varphi\rangle = 0$ .

One could also derive Eqs. (6.137) and (6.138) directly from the anti-commutation relations

$$[a_\alpha, a_\beta]_+ = [a_\alpha^+, a_\beta^+]_+ = 0; \quad [a_\alpha, a_\beta^+]_+ = \delta_{\alpha\beta} \quad (6.139)$$

as was done in previous sections for the  $a_\alpha$ 's of the harmonic-oscillator system. But for the Fermi case there does not appear to be any *a priori* reason for postulating Eq. (6.139). (Remember, for oscillators the corresponding commutation rules followed from the canonical quantization procedure.) One may rather consider Eq. (6.139) as derived from the antisymmetrization postulate for fermions.

Let us return to the general case where Eqs. (6.126) through (6.132) apply. One advantage of deriving them in such a general form is that we are not tied down to a particular basis of states. Suppose we use a basis of momentum eigenstates,  $|\mathbf{p}\rangle$ . Because  $\langle \mathbf{p} | \mathbf{p}' \rangle = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}')$  we have

$$\begin{aligned} [a(\mathbf{p}), a^+(\mathbf{p}') ]_{-\zeta} &= (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}'), \\ [a(\mathbf{p}), a(\mathbf{p}') ]_{-\zeta} &= [a^+(\mathbf{p}), a^+(\mathbf{p}') ]_{-\zeta} = 0. \end{aligned} \quad (6.140)$$

From the vacuum state we can construct the other states by

$$|\mathbf{p}_1, \dots, \mathbf{p}_n\rangle = a^+(\mathbf{p}_1) \cdots a^+(\mathbf{p}_n) |\text{vac}\rangle. \quad (6.141)$$

If we use a basis of position eigenstates  $|x\rangle$ , then since  $\langle x|x'\rangle = \delta^3(x - x')$ ,

$$[a(x), a^+(x')]_{-\zeta} = \delta^3(x - x'), \quad (6.142)$$

$$|x_1, \dots, x_n\rangle = a^+(x_1) \cdots a^+(x_n)|\text{vac}\rangle. \quad (6.143)$$

If we use a basis of hydrogen-atom energy eigenstates  $|nlm\rangle$ , then  $[a(nlm), a^+(n'l'm')]\_{-\zeta} = \delta_{nn'} \delta_{ll'} \delta_{mm'}$ , and so on.

How do the creation and destruction operators change when we make a change of basis? This question is easily answered by noting that if

$$|\chi\rangle = \alpha|\psi\rangle + \beta|\varphi\rangle, \quad (6.144)$$

then

$$\begin{aligned} a^+(\chi) &= \alpha a^+(\psi) + \beta a^+(\varphi), \\ a(\chi) &= \alpha^* a(\psi) + \beta^* a(\varphi), \end{aligned} \quad (6.145)$$

This means that creation operators “transform” like kets, whereas destruction operators “transform” like bras (because  $\langle\chi| = \alpha^*\langle\psi| + \beta^*\langle\varphi|$ ). Equation (6.145) are readily generalized to infinite series and integrals. Now if we change, for example, from position to momentum representation, so that

$$\begin{aligned} |p\rangle &= \int d^3x |x\rangle \langle x|p\rangle = \int d^3x |x\rangle e^{ip \cdot x}, \\ |x\rangle &= \int \frac{d^3p}{(2\pi)^3} |p\rangle \langle p|x\rangle = \int \frac{d^3p}{(2\pi)^3} |p\rangle e^{-ip \cdot x}, \end{aligned} \quad (6.146)$$

the creation operators are related by

$$\begin{aligned} a^+(p) &= \int d^3x a^+(x) e^{ip \cdot x}, \\ a^+(x) &= \int \frac{d^3p}{(2\pi)^3} a^+(p) e^{-ip \cdot x}. \end{aligned} \quad (6.147)$$

To relate the destruction operators  $a(p)$  and  $a(x)$ , simply take the Hermitian adjoint of Eq. (6.147). One proceeds in a similar way for any other change of basis.

**Exercise:** Suppose we have a complete orthonormal set of states  $|\alpha\rangle$ , and we let the “wave functions” of these states be  $\langle x|\alpha\rangle = u_\alpha(x)$ . Write down the formulas for  $a^+(x)$  and  $a(x)$  in terms of  $a_\alpha^+$  and  $a_\alpha$ , and vice versa.

## 6.8 THE HAMILTONIAN AND OTHER OPERATORS

In the last section we developed a method for describing systems containing many Bose or Fermi particles, and we defined creation and destruction operators

for the particle states. We will now show that these operators have other uses than merely creating and destroying states.

Suppose  $A^{(1)}$  is an operator that acts only on one-particle states. We wish to find an operator  $A$  that represents the “sum of  $A^{(1)}$  over all of the particles.” That is, for any  $n$ -particle state

$$|\psi\rangle = |\psi_1, \dots, \psi_n\rangle = |\psi_1\rangle \times \dots \times |\psi_n\rangle \quad (6.148)$$

we want  $A|\psi\rangle$  to satisfy

$$A|\psi\rangle = A^{(1)}|\psi_1\rangle \times |\psi_2\rangle \times \dots \times |\psi_n\rangle + |\psi_1\rangle \times A^{(1)}|\psi_2\rangle \times \dots \times |\psi_n\rangle + \dots + |\psi_1\rangle \times |\psi_2\rangle \times \dots \times A^{(1)}|\psi_n\rangle. \quad (6.149)$$

To see what this means, suppose each  $|\psi_i\rangle$  is an eigenstate of  $A^{(1)}$  with eigenvalue  $a_i$ . Then Eq. (6.149) implies that

$$A|\psi\rangle = (a_1 + \dots + a_n)|\psi\rangle. \quad (6.150)$$

For example, if  $A^{(1)}$  is the single-particle Hamiltonian, then  $A$  is the total energy (ignoring mutual interactions, which we shall consider later in this section). If  $A^{(1)}$  is the momentum operator for a single particle, then  $A$  is the total momentum. If  $A^{(1)} = 1^{(1)}$  (the unit operator on one-particle states), then  $A = N$ , the “number-of-particles operator.”

The desired operator  $A$  is easy to find. We first find it for the special case  $A^{(1)} = |\alpha\rangle\langle\beta|$ . In this case Eq. (6.149) becomes

$$A|\psi\rangle = \langle\beta|\psi_1\rangle|\alpha, \psi_2, \dots, \psi_n\rangle + \langle\beta|\psi_2\rangle|\psi_1, \alpha, \dots, \psi_n\rangle + \dots + \langle\beta|\psi_n\rangle|\psi_1, \psi_2, \dots, \alpha\rangle. \quad (6.151)$$

Now look back at Eq. (6.131) and notice that when  $\varphi_2 = \alpha$  and  $\varphi_1 = \beta$  we have

$$a^+(\alpha)a(\beta)|\psi\rangle = \sum_{k=1}^n \zeta^{k-1} \langle\beta|\psi_k\rangle |\alpha_1\psi_1, \dots, (\text{no } \psi_k), \dots, \psi_n\rangle. \quad (6.152)$$

But

$$\zeta^{k-1} |\alpha, \psi_1, \dots, (\text{no } \psi_k), \dots, \psi_n\rangle = |\psi_1, \dots, \psi_{k-1}, \alpha, \psi_{k+1}, \dots, \psi_n\rangle$$

due to the symmetry property of the  $n$ -particle state. Using this equation in Eq. (6.152) and comparing it with Eq. (6.151) we find

$$A = a^+(\alpha)a(\beta) \quad \text{when} \quad A^{(1)} = |\alpha\rangle\langle\beta|. \quad (6.153)$$

The generalization of Eq. (6.153) for an arbitrary one-particle operator  $A^{(1)}$  is immediate. We choose a basis—any basis—of one-particle state  $|\alpha\rangle$ , and write

$$A^{(1)} = \sum_{\alpha, \beta} |\alpha\rangle\langle\alpha|A^{(1)}|\beta\rangle\langle\beta| = \sum_{\alpha, \beta} A_{\alpha\beta}^{(1)}|\alpha\rangle\langle\beta|. \quad (6.154)$$

Then, from Eq. (6.153) and linearity,

$$A = \sum_{\alpha, \beta} A_{\alpha\beta}^{(1)} a^+(\alpha) a(\beta). \quad (6.155)$$

As a first example we consider  $A^{(1)} = 1^{(1)}$ , so that  $A = N$ , the operator for the number of particles. Using various bases we have

$$\begin{aligned} 1^{(1)} &= \sum_{\alpha} |\alpha\rangle\langle\alpha| \\ &= \int d^3x |x\rangle\langle x| \\ &= \int \frac{d^3p}{(2\pi)^3} |p\rangle\langle p| \end{aligned} \quad (6.156)$$

from which we can immediately write

$$\begin{aligned} N &= \sum_{\alpha} a_{\alpha}^+ a_{\alpha} \\ &= \int d^3x a^+(x) a(x) \\ &= \int \frac{d^3p}{(2\pi)^3} a^+(p) a(p). \end{aligned} \quad (6.157)$$

Next, consider the momentum operator. Because

$$\begin{aligned} \mathbf{P}^{(1)} &= \int \frac{d^3p}{(2\pi)^3} \mathbf{p} |p\rangle\langle p| \\ &= \int d^3x |x\rangle\langle x| \frac{1}{i} \nabla \langle x| \end{aligned} \quad (6.158)$$

we have for the total momentum

$$\begin{aligned} \mathbf{P} &= \int \frac{d^3p}{(2\pi)^3} \mathbf{p} a^+(p) a(p) \\ &= \int d^3x a^+(x) \frac{1}{i} \nabla a(x). \end{aligned} \quad (6.159)$$

(Compare the first of these expressions for  $\mathbf{P}$  with Eq. (6.100), another expression for  $\mathbf{P}$ .)

Finally, suppose the Hamiltonian for a single particle is

$$H^{(1)} = \frac{\mathbf{P}^2}{2m} + V(x), \quad (6.160)$$

where  $x$  is the position operator. In coordinate representation,

$$\langle x|H^{(1)}|x'\rangle = -\frac{1}{2m}\nabla^2\delta^3(x-x') + V(x)\delta^3(x-x'), \quad (6.161)$$

so that

$$\begin{aligned} H &= \int d^3x \int d^3x' \left[ -\frac{1}{2m}\nabla^2\delta^3(x-x') + V(x)\delta^3(x-x') \right] a^+(x)a(x') \\ &= \int d^3x a^+(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] a(x). \end{aligned} \quad (6.162)$$

In momentum representation\*

$$\begin{aligned} \langle p|H^{(1)}|p'\rangle &= \frac{p^2}{2m}(2\pi)^3\delta^3(p-p') + \int d^3x e^{-i\mathbf{p}\cdot\mathbf{x}}V(x)e^{i\mathbf{p}'\cdot\mathbf{x}} \\ &= \frac{p^2}{2m}(2\pi)^3\delta^3(p-p') + \tilde{V}(p-p'), \end{aligned} \quad (6.163)$$

where

$$\tilde{V}(q) = \int d^3x V(x)e^{-i\mathbf{q}\cdot\mathbf{x}}. \quad (6.164)$$

Therefore

$$\begin{aligned} H &= \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{2m} a^+(p)a(p) + \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} \tilde{V}(p-p')a^+(p)a(p') \\ &= \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{2m} a^+(p)a(p) + \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \tilde{V}(q)a^+(p+q)a(p). \end{aligned} \quad (6.165)$$

The term  $\tilde{V}(q)a^+(p+q)a(p)$  annihilates a particle of momentum  $p$  and recreates it with momentum  $p+q$ , the amplitude for this process being  $\tilde{V}(q)$ . If we use a basis of eigenstate  $|\alpha\rangle$  of  $H^{(1)}$ , so that

$$\langle\alpha|H^{(1)}|\beta\rangle = E_\alpha\delta_{\alpha\beta} \quad (6.166)$$

then

$$H = \sum_\alpha E_\alpha a_\alpha^+ a_\alpha, \quad (6.167)$$

which is what we had for phonons with  $E_\alpha = \hbar\omega_\alpha$ .

\* The second term is obtained by noting that

$$V(X_p) = \int d^3x V(x)|x\rangle\langle x|$$

and putting this between states  $\langle p|$  and  $|p'\rangle$ .

All of these expressions for  $H$  can be derived from each other using the formulas relating  $a^+(\mathbf{x})$  and  $a^+(\mathbf{p})$ , and so on, described at the end of Section 6.7. But it is often simplest to obtain such expressions directly from the single-particle Hamiltonians, as we have done here.

The density of particles (that is, number per unit volume) at the point  $\mathbf{x}$  is given by the operator

$$\rho(\mathbf{x}) = a^+(\mathbf{x})a(\mathbf{x}) \quad (6.168)$$

(which corresponds to the one-particle operator  $|\mathbf{x}\rangle\langle\mathbf{x}|$ ). Thus the number-of-particles operator in Eq. (6.157) may be written as

$$N = \int d^3\mathbf{x}\rho(\mathbf{x}),$$

and the potential-energy term in Eq. (6.162) as

$$V = \int d^3\mathbf{x}V(\mathbf{x})\rho(\mathbf{x}).$$

This last equation represents the integral of the potential energy weighted by the density.

So far we have described a system of *independent* particles, each particle being (possibly) acted on by an external potential but no two particles influencing each other. Suppose, however, that there is an additional potential  $V^{(2)}(\mathbf{x}_i, \mathbf{x}_j)$  between any two particles at  $\mathbf{x}_i$  and  $\mathbf{x}_j$  (giving rise to a “two-body” force). We assume that  $V^{(2)}(\mathbf{x}_i, \mathbf{x}_j) = V^{(2)}(\mathbf{x}_j, \mathbf{x}_i)$ . On two-particle states the operator is then

$$V^{(2)} = \frac{1}{2} \int d^3\mathbf{x} \int d^3\mathbf{y} |\mathbf{x}, \mathbf{y}\rangle V^{(2)}(\mathbf{x}, \mathbf{y}) \langle\mathbf{x}, \mathbf{y}|, \quad (6.169)$$

as can be verified by applying it to a two-particle state  $|\mathbf{x}_1, \mathbf{x}_2\rangle$ . We now want an operator  $V$  on the whole multiparticle space such that

$$\begin{aligned} V|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle &= \sum_{i < j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j)|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle \\ &= \frac{1}{2} \sum_{i \neq j} V^{(2)}(\mathbf{x}_i, \mathbf{x}_j)|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle. \end{aligned} \quad (6.170)$$

Looking at Eq. (6.169) and noticing that  $a^+(\mathbf{x})a^+(\mathbf{y})$  creates the state  $|\mathbf{x}, \mathbf{y}\rangle$ , whereas  $a(\mathbf{y})a(\mathbf{x})$  destroys the same state, we might guess that

$$V = \frac{1}{2} \int d^3\mathbf{x} \int d^3\mathbf{y} a^+(\mathbf{x})a^+(\mathbf{y})V^{(2)}(\mathbf{x}, \mathbf{y})a(\mathbf{y})a(\mathbf{x}). \quad (6.171)$$

This is in fact correct, as can be verified by applying  $V$  to  $|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle$ . Using Eq. (6.127) twice, we have

$$\begin{aligned} a(\mathbf{y})a(\mathbf{x})|\mathbf{x}_1 \cdots \mathbf{x}_n\rangle &= a(\mathbf{y}) \sum_{k=1}^n \zeta^{k-1} \delta^3(\mathbf{x} - \mathbf{x}_k) |\mathbf{x}_1 \cdots (\text{no } \mathbf{x}_k) \cdots \mathbf{x}_n\rangle \\ &= \sum_{k=1}^n \zeta^{k-1} \delta^3(\mathbf{x} - \mathbf{x}_k) \sum_{\substack{j=1 \\ j \neq k}}^n \eta_{jk} \delta^3(\mathbf{y} - \mathbf{x}_j) |\mathbf{x}_1 \cdots (\text{no } \mathbf{x}_k, \mathbf{x}_j) \cdots \mathbf{x}_n\rangle, \end{aligned}$$

where

$$\eta_{jk} = \begin{cases} \zeta^{j-1} & \text{if } j < k \\ \zeta^j & \text{if } j > k \end{cases}$$

Then

$$\begin{aligned} a^+(\mathbf{x})a^+(\mathbf{y})a(\mathbf{y})a(\mathbf{x})|\mathbf{x}_1, \dots, \mathbf{x}_n\rangle &= \sum_{j \neq k} \zeta^{k-1} \eta_{jk} \delta^3(\mathbf{x} - \mathbf{x}_k) \delta^3(\mathbf{y} - \mathbf{x}_j) |\mathbf{x}, \mathbf{y}, \mathbf{x}_1, \dots, (\text{no } \mathbf{x}_k, \mathbf{x}_j), \dots, \mathbf{x}_n\rangle \\ &= \sum_{j \neq k} \zeta^{k-1} \eta_{jk} \delta^3(\mathbf{x} - \mathbf{x}_k) \delta^3(\mathbf{y} - \mathbf{x}_j) |\mathbf{x}_k, \mathbf{x}_j, \dots, (\text{no } \mathbf{x}_k, \mathbf{x}_j), \dots, \mathbf{x}_n\rangle \\ &= \sum_{j \neq k} \delta^3(\mathbf{x} - \mathbf{x}_k) \delta^3(\mathbf{y} - \mathbf{x}_j) |\mathbf{x}_1, \dots, \mathbf{x}_n\rangle. \end{aligned}$$

Multiplying by  $\frac{1}{2}V^{(2)}(\mathbf{x}, \mathbf{y})$  and integrating over  $\mathbf{x}$  and  $\mathbf{y}$ , we find that  $V$  as given by Eq. (6.171) indeed satisfies Eq. (6.170).

In view of Eq. (6.168) and the remarks following it, we might expect that the mutual interaction could also be described in terms of the particle density by the operator

$$V' = \frac{1}{2} \int d^3\mathbf{x} \int d^3\mathbf{y} V^{(2)}(\mathbf{x}, \mathbf{y}) \rho(\mathbf{x}) \rho(\mathbf{y}). \quad (6.172)$$

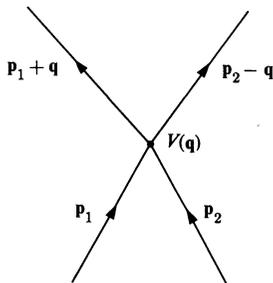
However,  $V'$  is not quite the same as  $V$ . To see the difference we write

$$\begin{aligned} \rho(\mathbf{x})\rho(\mathbf{y}) &= a^+(\mathbf{x})a(\mathbf{x})a^+(\mathbf{y})a(\mathbf{y}) \\ &= \zeta a^+(\mathbf{x})a^+(\mathbf{y})a(\mathbf{x})a(\mathbf{y}) + \delta^3(\mathbf{x} - \mathbf{y})a^+(\mathbf{x})a(\mathbf{y}) \\ &= a^+(\mathbf{x})a^+(\mathbf{y})a(\mathbf{y})a(\mathbf{x}) + \delta^3(\mathbf{x} - \mathbf{y})a^+(\mathbf{x})a(\mathbf{x}), \end{aligned}$$

so that

$$V' = V + \frac{1}{2} \int d^3\mathbf{x} V^{(2)}(\mathbf{x}, \mathbf{x}) \rho(\mathbf{x}). \quad (6.173)$$

Thus  $V'$  contains an extra term, which may be interpreted as a self-energy; it contributes even when there is only one particle present. The true mutual interaction  $V$  is zero unless there are two or more particles. We want only the



**Fig. 6.1** Operator  $V$  adds momentum  $q$  to one particle and subtracts it from the other.

mutual interaction, because any self-energy (if it exists in nature) can be included in the Hamiltonian of Eq. (6.162). Besides, for many potentials (for example, the Coulomb potential),  $V'$  is infinite and is not what we would consider to be the true energy.

If we express  $V$  in momentum representation, using Eqs. (6.171) and (6.147), and assume

$$V^{(2)}(\mathbf{x}, \mathbf{y}) = V(\mathbf{x} - \mathbf{y}) = V(\mathbf{y} - \mathbf{x}), \quad (6.174)$$

we arrive at

$$V = \frac{1}{2} \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \int \frac{d^3 \mathbf{p}'}{(2\pi)^3} \tilde{V}(\mathbf{q}) a^+(\mathbf{p} + \mathbf{q}) a^+(\mathbf{p}' - \mathbf{q}) a(\mathbf{p}') a(\mathbf{p}). \quad (6.175)$$

Here  $\tilde{V}(\mathbf{q})$  is as defined in Eq. (6.164) (in proving Eq. (6.175) we use  $\tilde{V}(\mathbf{q}) = \tilde{V}(-\mathbf{q})$ , because  $V(\mathbf{x}) = V(-\mathbf{x})$ ). Note that

$$V|p_1, p_2\rangle = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \tilde{V}(\mathbf{q}) |p_1 + \mathbf{q}, p_2 - \mathbf{q}\rangle,$$

which says that  $V$  adds momentum  $\mathbf{q}$  to one particle and subtracts it from the other with amplitude  $V(\mathbf{q})$ . This process is denoted by the diagram in Fig. 6.1. The total momentum is conserved, as we would expect, because Eq. (6.174) implies that the mutual interaction is invariant under translations.

The Hamiltonian and mutual interactions described here all conserve the total number of particles (see the exercise at the end of Section 6.5).

## 6.9 GROUND STATE FOR A FERMION SYSTEM

In this section we will consider fermions, so that the results of Sections 6.7 and 6.8 apply with  $\zeta = -1$ . Suppose we know the eigenstates and eigenvalues of the single-particle Hamiltonians,  $H^{(1)}$ :

$$H^{(1)}|\alpha\rangle = E_\alpha|\alpha\rangle, \quad (\alpha = 1, 2, 3, \dots). \quad (6.176)$$

Then, ignoring mutual interactions, we have for the multiparticle Hamiltonian:

$$H = \sum_{\alpha} E_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}. \quad (6.177)$$

Every state may be built up from the vacuum state by applying creation operators:

$$|\alpha_1, \dots, \alpha_n\rangle = a_{\alpha_1}^{\dagger} \dots a_{\alpha_n}^{\dagger} |\text{vac}\rangle. \quad (6.178)$$

(Both sides vanish unless the  $\alpha_i$  are all distinct.)

It is often inconvenient to refer everything to the vacuum state, as in Eq. (6.178). In practice we may be considering states that differ from some "ground" state only by the presence or absence of a few particles. Suppose there are  $G$  particles present. Assume that the energy levels are ordered such that

$$E_1 \leq E_2 \leq E_3 \leq \dots$$

Then the state of lowest energy is

$$|\text{gnd}\rangle = |1, \dots, G\rangle = a_1^{\dagger} \dots a_G^{\dagger} |\text{vac}\rangle, \quad (6.179)$$

which we call the *ground state*; its energy is

$$E_{\text{gnd}} = E_1 + \dots + E_G. \quad (6.180)$$

Any other  $G$ -particle state will have some of the levels  $1, \dots, G$  unoccupied and some higher levels occupied. It is convenient to use  $|\text{gnd}\rangle$  as a reference, describing the removal of a particle from  $1, \dots, G$  as the creation of a "hole." Particles in the levels  $G + 1, G + 2, \dots$  are still called "particles." If a particle is excited from the level  $\alpha$  to the level  $\beta$  ( $\alpha \leq G \leq \beta$ ), then we say that a hole with energy  $-E_{\alpha}$  has been created as well as a particle with energy  $E_{\beta}$ .

The concept of holes may be formulated mathematically as follows: Define

$$b_{\alpha} = a_{\alpha}^{\dagger} \quad \text{for } \alpha \leq G. \quad (6.181)$$

From the anticommutation relations in Eq. (6.139) we have, if  $\alpha, \alpha' > G$  and  $\beta, \beta' \leq G$ ,

$$\begin{aligned} [a_{\alpha}, a_{\alpha'}]_{+} &= [a_{\alpha}, b_{\beta}]_{+} = [b_{\beta}, b_{\beta'}]_{+} = 0, \\ [a_{\alpha}, a_{\alpha'}^{\dagger}]_{+} &= \delta_{\alpha\alpha'}; [b_{\beta}, b_{\beta'}^{\dagger}]_{+} = \delta_{\beta\beta'}, \\ [a_{\alpha}, b_{\beta}^{\dagger}]_{+} &= 0. \end{aligned} \quad (6.182)$$

Thus the operators  $a_{\alpha}^{\dagger}$  ( $\alpha > G$ ) and  $b_{\alpha}^{\dagger}$  ( $\alpha \leq G$ ) behave like creation operators. We can now express the states in the form

$$|\alpha_1, \dots, \alpha_m, \beta_1, \dots, \beta_n, \text{gnd}\rangle \equiv a_{\alpha_1}^{\dagger} \dots a_{\alpha_m}^{\dagger} b_{\beta_1}^{\dagger} \dots b_{\beta_n}^{\dagger} |\text{gnd}\rangle \quad (6.183)$$

( $\alpha_i > G, \beta_i \leq G$ ). We call this a state with  $m$  particles and  $n$  holes. The ground state acts like a vacuum state in that

$$a_\alpha |\text{gnd}\rangle = b_\beta |\text{gnd}\rangle = 0. \quad (6.184)$$

The Hamiltonian of Eq. (6.177) may be written in the form

$$\begin{aligned} H &= \sum_{\alpha > G} E_\alpha a_\alpha^\dagger a_\alpha + \sum_{\alpha \leq G} E_\alpha b_\alpha b_\alpha^\dagger \\ &= \sum_{\alpha > G} E_\alpha a_\alpha^\dagger a_\alpha + \sum_{\alpha \leq G} E_\alpha (-b_\alpha^\dagger b_\alpha + 1) \\ &= E_{\text{gnd}} + \sum_{\alpha > G} E_\alpha a_\alpha^\dagger a_\alpha - \sum_{\alpha \leq G} E_\alpha b_\alpha^\dagger b_\alpha, \end{aligned} \quad (6.185)$$

so that the energy of a hole in state  $\alpha$  is  $-E_\alpha$ . In other words, it takes an energy  $-E_\alpha$  to create the hole. The number-of-particles operator is

$$\begin{aligned} N &= \sum_\alpha a_\alpha^\dagger a_\alpha \\ &= \sum_{\alpha > G} a_\alpha^\dagger a_\alpha + \sum_{\alpha \leq G} (-b_\alpha^\dagger b_\alpha + 1) \\ &= G + \sum_{\alpha > G} a_\alpha^\dagger a_\alpha - \sum_{\alpha \leq G} b_\alpha^\dagger b_\alpha; \end{aligned} \quad (6.186)$$

thus a hole counts as  $-1$ . The number of particles and holes outside the ground state (that is, the number  $m + n$  in Eq. (6.183)) is given by the operator

$$N' = \sum_{\alpha > G} a_\alpha^\dagger a_\alpha + \sum_{\alpha \leq G} b_\alpha^\dagger b_\alpha, \quad (6.187)$$

which counts a hole as  $+1$  and the ground state as nothing.

Suppose now that a perturbation is applied to the system in the form of an external potential

$$U = \sum_{\alpha, \beta} U_{\alpha\beta}^{(1)} a_\alpha^\dagger a_\beta, \quad (6.188)$$

where we assume that the single-particle potential  $U_{\alpha\beta}^{(1)}$  may be nondiagonal. Then

$$\begin{aligned} U &= \sum_{\substack{\alpha > G \\ \beta > G}} U_{\alpha\beta}^{(1)} a_\alpha^\dagger a_\beta + \sum_{\substack{\alpha > G \\ \beta \leq G}} U_{\alpha\beta}^{(1)} a_\alpha^\dagger b_\beta^\dagger \\ &\quad + \sum_{\substack{\alpha \leq G \\ \beta > G}} U_{\alpha\beta}^{(1)} b_\alpha a_\beta - \sum_{\substack{\alpha \leq G \\ \beta \leq G}} U_{\alpha\beta}^{(1)} b_\beta^\dagger b_\alpha + \sum_{\alpha \leq G} U_{\alpha\alpha}^{(1)}. \end{aligned} \quad (6.189)$$

The first and fourth terms of this equation modify the energies of the particles and holes, respectively, and the fifth term modifies the ground-state energy. The second term creates particle-hole pairs, and the third term destroys them. Note that  $N$ , as given by Eq. (6.186), is conserved, whereas  $N'$ , as defined in Eq. (6.187), is not.

Suppose further that there is a mutual interaction, a two-body potential of the form described in Section 6.8:

$$V = \sum_{\alpha, \beta, \gamma, \delta} V_{\alpha\beta, \gamma\delta}^{(2)} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}. \quad (6.190)$$

As in Eq. (6.189), we can express  $V$  in terms of  $a_{\alpha}$  ( $\alpha > G$ ) and  $b_{\alpha}$  ( $\alpha \leq G$ ), and then use the anticommutation rules of Eq. (6.182) to write  $V$  in a form such that in every term all of the creation operators are to the left of all of the destruction operators. Such terms are called “normal products.” The result will be a number of terms involving four operators, plus other terms that can be lumped into  $U$  or added to  $E_{\text{gnd}}$ .

### 6.10 HAMILTONIAN FOR A PHONON-ELECTRON SYSTEM

Now we will consider, as an application of the creation and destruction operator formalism, the interaction between the electrons and lattice vibrations in a crystal. It is this interaction (as well as the presence of crystal impurities and imperfections) that accounts for the finite conductivity of metals under most conditions. (One might otherwise expect from the band theory of metals that, once an electron got into an unfilled band, it would move unhindered, resulting in infinite conductivity.) We will show how the Hamiltonian is derived and written in terms of creation and destruction operators.

We start with the electron in a lattice with no vibrations. Let  $N = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$  (where  $n_1, n_2, n_3$  are integers) describe the positions of the nuclei. The potential  $V(\mathbf{x})$  felt by an electron in the lattice is periodic and has the form

$$V_1(\mathbf{x}) = \sum_N V_0(\mathbf{x} - N). \quad (6.191)$$

The Hamiltonian for a system of independent electrons in the lattice is, from Section 6.8,

$$H_{\text{el}} = \int d^3x a^{\dagger}(\mathbf{x}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_1(\mathbf{x}) \right] a(\mathbf{x}). \quad (6.192)$$

Now, suppose we have solved this part of the problem and know the one-particle eigenstates  $|\alpha\rangle$  and eigenvalues  $E_{\alpha}$ . Denoting  $\langle x|\alpha\rangle$  by  $\varphi_{\alpha}(x)$  we have

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_1(\mathbf{x}) \right] \varphi_{\alpha}(\mathbf{x}) = E_{\alpha} \varphi_{\alpha}(\mathbf{x}). \quad (6.193)$$

Then we can express the electron Hamiltonian as

$$H_{\text{el}} = \sum_{\alpha} E_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}. \quad (6.194)$$

Because

$$|x\rangle = \sum_{\alpha} |\alpha\rangle \langle \alpha|x\rangle = \sum_{\alpha} |\alpha\rangle \varphi_{\alpha}^*(x)$$

we have

$$a^+(\mathbf{x}) = \sum_{\alpha} a_{\alpha}^+ \varphi_{\alpha}^*(\mathbf{x}) \quad (6.195)$$

and similarly

$$a_{\alpha}^+ = \int d^3x a^+(\mathbf{x}) \varphi_{\alpha}(\mathbf{x}). \quad (6.196)$$

To obtain relations between the destruction operators, simply take the Hermitian adjoints of Eqs. (6.195) and (6.196).

If, as in Section 6.9, we refer all states to a ground state (called the “electron sea”), which is normally filled, then in the notation of that section,

$$H_{\text{el}} = E_{\text{gnd}} + \sum_{\alpha > G} E_{\alpha} a_{\alpha}^+ a_{\alpha} - \sum_{\alpha \leq G} E_{\alpha} b_{\alpha}^+ b_{\alpha}. \quad (6.197)$$

In what follows we shall ignore the ground-state energy, so that the electron Hamiltonian becomes  $H'_{\text{el}}$ :

$$H'_{\text{el}} = \sum_{\alpha > G} E_{\alpha} a_{\alpha}^+ a_{\alpha} - \sum_{\alpha \leq G} E_{\alpha} b_{\alpha}^+ b_{\alpha}. \quad (6.198)$$

Note that, in terms of electron and hole operators, Eq. (6.195) and its adjoint become

$$\begin{aligned} a^+(\mathbf{x}) &= \sum_{\alpha > G} a_{\alpha}^+ \varphi_{\alpha}^*(\mathbf{x}) + \sum_{\alpha \leq G} b_{\alpha} \varphi_{\alpha}^*(\mathbf{x}), \\ a(\mathbf{x}) &= \sum_{\alpha > G} a_{\alpha} \varphi_{\alpha}(\mathbf{x}) + \sum_{\alpha \leq G} b_{\alpha}^+ \varphi_{\alpha}(\mathbf{x}). \end{aligned} \quad (6.199)$$

Consider next the lattice vibrations. For each  $N$  let  $Z_N$  be the displacement of the corresponding nucleus from its equilibrium position  $N$ . The  $Z_N$  form a set of coordinates for a system of harmonic oscillators. The procedure for finding the normal modes and quantizing this system is similar to the field quantization of Section 6.6, except that Fourier transforms are replaced by Fourier series, with the “momentum”  $\mathbf{k}$  of the phonons running over a limited region. The normal coordinates  $q_{\mathbf{k},a}$  are related to the  $Z_N$  by equations of the following form (assuming for simplicity that “ $a$ ” runs from 1 to 3 as in the case of one atom per unit cell of the crystal):

$$\begin{aligned} \frac{q_{\mathbf{k},a}}{\sqrt{V}} &= \sum_N e^{-i\mathbf{k} \cdot \mathbf{N}} \mathbf{e}_{\mathbf{k},a}^* \cdot \mathbf{Z}_N, \\ \mathbf{Z}_N &= \int_K \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{a=1}^3 \mathbf{e}_{\mathbf{k},a} e^{i\mathbf{k} \cdot \mathbf{N}} \frac{q_{\mathbf{k},a}}{\sqrt{V}}. \end{aligned} \quad (6.200)$$

Here the region of integration is  $K = \{\mathbf{k} | -\pi \leq \mathbf{k} \cdot \mathbf{a}_i \leq \pi; i = 1, 2, 3\}$ ;  $V = |\mathbf{a}_1 \times \mathbf{a}_2 \cdot \mathbf{a}_3|$  is the volume of the unit cell of the crystal lattice (recall that the  $\mathbf{a}_i$  are vectors describing the periodicity of the lattice), and  $\mathbf{e}_{\mathbf{k},a}$  ( $a = 1, 2, 3$ )

form an orthonormal basis of 3-space for each  $\mathbf{k}$  (in that  $\mathbf{e}_{\mathbf{k},a}^* \cdot \mathbf{e}_{\mathbf{k},b} = \delta_{ab}$ ), chosen so that the mode  $(\mathbf{k}, a)$  is a normal mode.

You should check the consistency of Eqs. (6.200) as an exercise. It is convenient to use the relation

$$V \int_{\mathbf{K}} \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{N} - \mathbf{N}')} = \delta_{\mathbf{N}, \mathbf{N}'},$$

and the easiest way to verify it is to make a change of variables  $\mathbf{r}_i = \mathbf{K} \cdot \mathbf{a}_i$ .  $\mathbf{N} - \mathbf{N}'$  can be written as

$$\sum_{i=1}^3 m_i \mathbf{a}_i,$$

where  $m_i$  are integers, so that  $\mathbf{K} \cdot (\mathbf{N} - \mathbf{N}') = \mathbf{m} \cdot \mathbf{r}$ , and the Jacobian of the transformation is

$$\left\| \frac{\partial \mathbf{k}}{\partial \mathbf{r}} \right\| = \frac{1}{\left\| \frac{\partial \mathbf{r}}{\partial \mathbf{k}} \right\|} = \frac{1}{V}.$$

Equations 6.200 are essentially a special case of Eqs. (1.28) and (1.29). The change of notation is

<u>Chapter 1</u>	<u>Chapter 6</u>
$Q_r(\mathbf{k})$	$\frac{q_{\mathbf{k},r}}{\sqrt{V}}$
$a_\alpha^r(k)$	The $\alpha$ th component of $\mathbf{e}_{\mathbf{k},r}$
$Z_{\alpha,N}$	The $\alpha$ th component of $\mathbf{Z}_N$
$\frac{V}{n}$	$V$

The normalization conventions used in Eq. (6.200) are convenient because, in the limit that the lattice approaches a continuum (i.e.,  $\mathbf{a}_i \rightarrow 0$ ),  $\mathbf{K}$  becomes all of momentum space and, letting  $\mathbf{x} = \mathbf{N}$ , we have

$$V \sum_{\mathbf{N}} \rightarrow \int d^3 \mathbf{x} \quad \text{and} \quad \frac{1}{V} \delta_{\mathbf{N}\mathbf{N}'} \rightarrow \delta^3(\mathbf{x} - \mathbf{x}'), \quad (6.201)$$

Thus we have obtained the normalization of Section 6.6 for a field  $\varphi(\mathbf{x})$ , where

$$\sqrt{M/V} \mathbf{Z}_N \rightarrow \varphi(\mathbf{x}).$$

Following the procedure of Section 6.6 we have an expression for  $Z_N$  in terms of creation and destruction operators:

$$Z_N = \int_K \frac{d^3k}{(2\pi)^3} \sum_a \sqrt{\frac{\hbar V}{2M\omega(k, a)}} [A(k, a)e^{ik \cdot N} e_{k,a} + A^+(k, a)e^{-ik \cdot N} e_{k,a}^*], \quad (6.202)$$

where

$$[A(k, a), A^+(k', a')] = (2\pi)^3 \delta^3(k - k') \delta_{aa'}. \quad (6.203)$$

$M$  is the mass of the vibrating atom, and  $\omega(k, a)$  is the frequency of the corresponding mode. The Hamiltonian for the oscillator system (apart from a constant term) is

$$H_{\text{osc}} = \int_K \frac{d^3k}{(2\pi)^3} \sum_a \hbar\omega(k, a) A^+(k, a) A(k, a). \quad (6.204)$$

(We have used  $A$  for the phonon operators\* to avoid confusion with the electron creation and destruction operators.)

Having written down Hamiltonians for the electrons and the phonons (lattice-vibration states), we now turn to the interaction between them. The potential energy of an electron in an undisturbed lattice was given by Eq. (6.191). If the nucleus at  $N$  is displaced by an amount  $Z_N$ , then the potential energy changes to

$$V_1(x) + \Delta V_1(x) = \sum_N V_0(x - N - Z_N), \quad (6.205)$$

where we have assumed that each atom in the crystal acts like a rigid body when it is displaced, so that the potential  $V_0$  arising from it is simply displaced by  $Z_N$ . (In practice, not all the electron shells around the nucleus move by the same amount, so that the potential changes its shape as well as being displaced; however, we shall ignore this fact.) The potential  $V_1(x)$  was already included in  $H_{\text{el}}$ . Writing

$$V_0(x - N - Z_N) \approx V_0(x - N) - Z_N \cdot \nabla V_0(x - N)$$

we have for the interaction energy (that is, the extra energy of the system due to displacement of the lattice):

$$\Delta V_1(x) = - \sum_N Z_N \cdot \nabla V_0(x - N). \quad (6.206)$$

---

\* Note that  $A^+(k, a)$  (as well as the state it creates) has the dimensions of  $(\text{length})^{3/2}$ , as do the corresponding operators for other particles in momentum representation.

For the many electron system the interaction Hamiltonian is

$$\begin{aligned} H_{\text{int}} &= \int d^3 \mathbf{x} \Delta V_1(\mathbf{x}) a^+(\mathbf{x}) a(\mathbf{x}) \\ &= \sum_{\alpha, \beta} V_{\alpha\beta} a_{\alpha}^+ a_{\beta}, \end{aligned} \quad (6.207)$$

where

$$\begin{aligned} V_{\alpha\beta} &= \int d^3 \mathbf{x} \varphi_{\alpha}^*(\mathbf{x}) \Delta V_1(\mathbf{x}) \varphi_{\beta}(\mathbf{x}) \\ &= - \sum_N \mathbf{Z}_N \cdot \int d^3 \mathbf{x} \varphi_{\alpha}^*(\mathbf{x}) \nabla V_0(\mathbf{x} - N) \varphi_{\beta}(\mathbf{x}). \end{aligned} \quad (6.208)$$

Now  $V_{\alpha\beta}$  is also an operator on phonon states, because  $\mathbf{Z}_N$  is an operator. Using Eq. (6.202) we get

$$V_{\alpha\beta} = \int_K \frac{d^3 \mathbf{k}}{(2\pi)^3} \sum_a [C_{\alpha\beta}(\mathbf{k}, a) A^+(\mathbf{k}, a) + C_{\beta\alpha}^*(\mathbf{k}, a) A(\mathbf{k}, a)], \quad (6.209)$$

where

$$C_{\alpha\beta}(\mathbf{k}, a) = - \sqrt{\frac{\hbar V}{2M\omega(\mathbf{k}, a)}} \mathbf{e}_{\mathbf{k}, a} \cdot \sum_N e^{i\mathbf{k} \cdot N} \int d^3 \mathbf{x} \varphi_{\alpha}^*(\mathbf{x}) \nabla V_0(\mathbf{x} - N) \varphi_{\beta}(\mathbf{x}). \quad (6.210)$$

Therefore,

$$H_{\text{int}} = \int_K \frac{d^3 \mathbf{k}}{(2\pi)^3} \sum_a \sum_{\alpha, \beta} [C_{\alpha\beta}(\mathbf{k}, a) A^+(\mathbf{k}, a) + C_{\beta\alpha}^*(\mathbf{k}, a) A(\mathbf{k}, a)] a_{\alpha}^+ a_{\beta}. \quad (6.211)$$

The total Hamiltonian of the system is

$$H = H_{\text{el}} + H_{\text{osc}} + H_{\text{int}}. \quad (6.212)$$

*Note:* The states of our system are of the form

$$|\alpha_1, \dots, \alpha_n; \mathbf{k}_1, a_1, \dots, \mathbf{k}_m, a_m\rangle \quad (n \text{ electrons and } m \text{ phonons}),$$

or, if we use the hole notation,

$$|\alpha_1, \dots, \alpha_m; \beta_1, \dots, \beta_n; \mathbf{k}_1, a_1, \dots, \mathbf{k}_p, a_p\rangle \quad (n \text{ electrons, } m \text{ holes, and } p \text{ phonons}).$$

The effect of a creation operator  $A^+(\mathbf{k}, a)$  on such a state may be defined as

$$A^+(\mathbf{k}, a) |\text{electrons, holes, } \mathbf{k}_1, a_1, \dots \rangle = |\mathbf{k}, a, \text{electrons, holes, } a_1, \dots \rangle,$$

which is in turn defined to be

$$|\text{electrons, holes, } \mathbf{k}, a, \mathbf{k}_1, a_1, \dots \rangle.$$

The result of this definition is that all phonon operators commute with all electron (and hole) operators. (In general, it is conventional to say that creation and destruction operators for different particles always commute unless the particles are both fermions. In the latter case it is convenient to define the operators to anticommute; then everything is consistent if we decide to call the particles different states of the same particle, as with the proton and neutron.)

If we write Eq. (6.211) in terms of electron and hole operators, we get an expression four times as long, involving terms of the form

$$\begin{aligned} A^+ a^+ a, & \quad A^+ a^+ b^+, & \quad A^+ b a, & \quad A^+ b b^+, \\ A a^+ a, & \quad A a^+ b^+, & \quad A b a, & \quad A b b^+. \end{aligned}$$

These terms represent the transition of an electron or hole from one state to another, or the creation or annihilation of an electron-hole pair. In each process a phonon is emitted or absorbed.

The foregoing derivation assumed that there is only one atom per unit cell of the crystal. However, the results are similar if there are more atoms (say  $A$ ) per unit cell, the only difference in the final result being that there are more phonon modes for a given  $\mathbf{k}$  ( $a$  running from 1 to  $3A$ ). As a simplification it may turn out that some of the modes do not “couple” to the electrons, that is, they do not influence the potential felt by the electrons; these modes are independent of the others and may be ignored. Such is the case in the Polaron Problem (Chapter 8), where only one phonon mode contributes for each  $\mathbf{k}$ .

## 6.11 PHOTON-ELECTRON INTERACTIONS

Suppose we shine light on the crystal of Section 6.10. What is the Hamiltonian now? To  $H$  we must add a term  $H_\gamma$  for the free electromagnetic field ( $\gamma$  refers to photons) and a term  $H_{e\gamma}$  for the interaction between electrons and photons.

For the free electromagnetic field, the classical Lagrangian density is

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}(\mathbf{E}^2 - c^2 \mathbf{B}^2) \\ &= \frac{1}{2}[\dot{A}^2 - c^2(\nabla \times \mathbf{A})^2] \\ &= \frac{1}{2} \left[ \dot{A}^2 - c^2 \sum_{i,j=1}^3 (\nabla_i A_j \nabla_i A_j - \nabla_i A_j \nabla_j A_i) \right], \end{aligned} \quad (6.213)$$

where  $A(x)$  satisfies the subsidiary condition\*

$$\nabla \cdot \mathbf{A} = 0. \quad (6.214)$$

\* We assume also that the scalar potential is zero. We are using “rationalized units,” but with  $\epsilon_0 = 1$ ; thus  $e^2/4\pi\hbar c \approx 1/137$  and  $\nabla \cdot \mathbf{E} = \rho$ ,  $\nabla \times \mathbf{B} = (1/c^2)(\mathbf{j} + \partial \mathbf{E}/\partial t)$ , etc.

The equation of motion resulting from the Lagrangian is

$$0 = c^2[\nabla^2 A - \nabla(\nabla \cdot A)] - \ddot{A} = c^2 \left[ \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right] A. \quad (6.215)$$

Carrying out the quantization procedure of Section 6.6, we find  $\omega(\mathbf{k}) = c|\mathbf{k}| = ck$ , and

$$A(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{r=1}^2 \sqrt{\frac{\hbar}{2ck}} [C(\mathbf{k}, r)e^{i\mathbf{k} \cdot \mathbf{x}} + C^+(\mathbf{k}, r)e^{-i\mathbf{k} \cdot \mathbf{x}}] \mathbf{e}_{\mathbf{k}, r}. \quad (6.216)$$

Here  $\mathbf{e}_{\mathbf{k}, r}$  ( $r = 1, 2$ ) are two unit vectors, perpendicular to each other and to  $\mathbf{k}$ , and  $C^+(\mathbf{k}, r)$  is the creation operator for a photon with momentum  $\hbar\mathbf{k}$  and polarization  $\mathbf{e}_{\mathbf{k}, r}$ :

$$[C(\mathbf{k}, r), C^+(\mathbf{k}', r')] = (2\pi)^3 \delta^3(\mathbf{k} - \mathbf{k}') \delta_{rr'}. \quad (6.217)$$

The Hamiltonian is

$$H_\gamma = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{r=1}^2 \hbar ck C^+(\mathbf{k}, r) C(\mathbf{k}, r). \quad (6.218)$$

To find the photon-electron interaction we replace the operator\*  $\mathbf{P}$  by  $\mathbf{P} + e\mathbf{A}(\mathbf{x})$  (the charge of the electron being  $-e$ ) in the single-particle Hamiltonian

$$H_{\text{el}}^{(1)} = \frac{\mathbf{P}^2}{2m} + V_1,$$

so that

$$\begin{aligned} H_{\text{el}}^{(1)} + H_{e\gamma}^{(1)} &= \frac{(\mathbf{P} + e\mathbf{A})^2}{2m} + V_1 \\ &= H_{\text{el}}^{(1)} + \frac{e}{2m} (\mathbf{P} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{P}) + \frac{e^2}{2m} A^2. \end{aligned} \quad (6.219)$$

Writing

$$A(X) = \int d^3\mathbf{x} A(\mathbf{x}) |x\rangle \langle x|, \quad (6.219')$$

we have

$$H_{e\gamma}^{(1)} = - \int d^3\mathbf{x} A(\mathbf{x}) \cdot \mathbf{j}^{(1)}(\mathbf{x}) + \frac{e^2}{2m} \int d^3\mathbf{x} A(\mathbf{x})^2 |x\rangle \langle x|, \quad (6.220)$$

\*  $\mathbf{P}$  and  $X$  are the electron momentum and position operators, and  $A(\mathbf{x})$  operates on photon states, so that  $A(X)$  (see Eq. (6.219')) operates on both photons and electrons.

where

$$\begin{aligned} \mathbf{j}^{(1)}(\mathbf{x}) &= -\frac{e}{2m} (\mathbf{P}|\mathbf{x}\rangle\langle\mathbf{x}| + |\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{P}) \\ &= -\frac{e\hbar}{2m} i[(\nabla|\mathbf{x}\rangle)\langle\mathbf{x}| - |\mathbf{x}\rangle(\nabla\langle\mathbf{x}|)]. \end{aligned} \quad (6.221)$$

Note that  $\mathbf{j}^{(1)}(\mathbf{x})$  is the charge  $-e$  multiplied by the probability current-density operator. The expectation value in any one-electron state  $|\psi\rangle$  is

$$\langle\psi|\mathbf{j}^{(1)}(\mathbf{x})|\psi\rangle = -\frac{e\hbar}{2m} i[\psi(\mathbf{x})\nabla\psi^*(\mathbf{x}) - \psi^*(\mathbf{x})\nabla\psi(\mathbf{x})].$$

By inspection of Eq. (6.220) we have, for the interaction between photons and systems of arbitrary numbers of electrons,

$$H_{ey} = -\int d^3\mathbf{x} A(\mathbf{x}) \cdot \mathbf{j}(\mathbf{x}) + \frac{e^2}{2m} \int d^3\mathbf{x} A(\mathbf{x})^2 a^+(\mathbf{x})a(\mathbf{x}), \quad (6.222)$$

where

$$\mathbf{j}(\mathbf{x}) = -\frac{e\hbar}{2m} i[\nabla a^+(\mathbf{x})a(\mathbf{x}) - a^+(\mathbf{x})\nabla a(\mathbf{x})] \quad (6.223)$$

is the electromagnetic current-density operator.

In Eq. (6.222),  $A(\mathbf{x})$  is itself an operator for each  $\mathbf{x}$ , given by Eq. (6.216). If we use Eq. (6.216) in Eq. (6.222), and also express  $a^+(\mathbf{x})$  in terms of  $a_\alpha^+$  using Eq. (6.195), we get terms involving

$$C^+(\mathbf{k}, r)a_\alpha^+ a_\beta, \quad C(\mathbf{k}, r)a_\alpha^+ a_\beta, \quad C(\mathbf{k}, r)C(\mathbf{k}', r')a_\alpha^+ a_\beta, \quad C(\mathbf{k}, r)C^+(\mathbf{k}', r')a_\alpha^+ a_\beta,$$

and so forth, which have interpretations similar to those of the phonon-electron interaction.

The electromagnetic current defined in Eq. (6.223) may be expressed in momentum representation as follows:

$$\mathbf{j}(\mathbf{x}) = -e \int \frac{d^3\mathbf{p}'}{(2\pi\hbar)^3} \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \frac{\mathbf{p}' + \mathbf{p}}{2m} a^+(\mathbf{p}')a(\mathbf{p})e^{-i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}/\hbar}. \quad (6.224)$$

This expression will be useful in Section 6.12.

## 6.12 FEYNMAN DIAGRAMS

A graphical method employing what have come to be called ‘‘Feynman diagrams’’ has proven to be very convenient in dealing with perturbation solutions of complicated Hamiltonians. These diagrams serve as a ‘‘bookkeeping’’ device to keep track of all the perturbation terms and a guide in writing down the value

of each term. (The diagrams assume their full power in the relativistic case, with which we are not concerned here.) To show how the method works we will consider the Hamiltonian for a single, otherwise free, electron interacting with the electromagnetic field:

$$H = H_{\text{free}} + H_{\text{int}},$$

where

$$H_{\text{free}} = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{\mathbf{p}^2}{2m} a^\dagger(\mathbf{p})a(\mathbf{p}) + \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{r=1}^2 ckA^+(\mathbf{k}, r)A(\mathbf{k}, r) \quad (6.225)$$

and

$$H_{\text{int}} = - \int d^3\mathbf{x} \mathbf{j}(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}) + \int d^3\mathbf{x} \frac{e^2}{2m} a^\dagger(\mathbf{x})a(\mathbf{x})\mathbf{A}(\mathbf{x})^2. \quad (6.226)$$

Here we denote the photon-creation operator by  $A^+(\mathbf{k}, r)$  instead of by  $C^+(\mathbf{k}, r)$ :

$$A(\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_{r=1}^2 \sqrt{\frac{1}{2ck}} [A(\mathbf{k}, r)e^{i\mathbf{k}\cdot\mathbf{x}} + A^+(\mathbf{k}, r)e^{-i\mathbf{k}\cdot\mathbf{x}}]e_{\mathbf{k},r}, \quad (6.227)$$

and  $\mathbf{j}(\mathbf{x})$  is given by Eqs. (6.223) and (6.224). In this section,  $\hbar = 1$ .

The states under consideration are of the form

$$|\mathbf{p}; \mathbf{k}_1, r_1; \dots; \mathbf{k}_n, r_n\rangle \quad (\text{one electron and } n \text{ photons}). \quad (6.228)$$

According to standard quantum-mechanical techniques, the transition amplitude  $M_{fi}$  for a transition from an initial state  $|i\rangle$  to a final state  $|f\rangle$  can be expressed in terms of the Hamiltonian (to second order) as follows:

$$(2\pi)^3\delta^3(\mathbf{p}_f - \mathbf{p}_i)M_{fi} = \langle f|H|i\rangle + \sum_n \frac{\langle f|H|n\rangle\langle n|H|i\rangle}{E_i - E_n + i\epsilon} + 0(H^3). \quad (6.229)$$

Cross sections and transition rates are proportional to the absolute square of the amplitude:

$$\text{Rate} = \sum_{\mathbf{f}} |M_{fi}|^2 (2\pi)^4 \delta^3(\mathbf{p}_f - \mathbf{p}_i) \delta(E_f - E_i).$$

In practice, the states  $|i\rangle$  and  $|f\rangle$  are usually states of the form given in Eq. (6.228), that is, states of particles of definite momentum. It is therefore convenient to express  $H_{\text{int}}$  in terms of the  $A(\mathbf{k}, r)$ , substituting Eq. (6.227) in Eq. (6.226), and to use Eq. (6.224) for  $\mathbf{j}(\mathbf{x})$ .

$$H_{\text{int}} = H_1 + H_2, \quad (6.230)$$

where

$$\begin{aligned}
 H_1 = & \int \frac{d^3 \mathbf{p}'}{(2\pi)^3} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \sum_r e^{\mathbf{p}' + \mathbf{p} \cdot \mathbf{e}_{\mathbf{k},r}} \frac{1}{\sqrt{2ck}} \\
 & \times [(2\pi)^3 \delta^3(\mathbf{p}' - \mathbf{p} - \mathbf{k}) a^+(\mathbf{p}') a(\mathbf{p}) A(\mathbf{k}, r) \\
 & + (2\pi)^3 \delta^3(\mathbf{p}' + \mathbf{k} - \mathbf{p}) a^+(\mathbf{p}') a(\mathbf{p}) A^+(\mathbf{k}, r)], \quad (6.231)
 \end{aligned}$$

and

$$\begin{aligned}
 H_2 = & \int \frac{d^3 \mathbf{p}'}{(2\pi)^3} \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \int \frac{d^3 \mathbf{k}'}{(2\pi)^3} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \sum_{r',r} \frac{e^2}{2m} \frac{1}{\sqrt{2ck'}\sqrt{2ck}} \mathbf{e}_{\mathbf{k}',r'} \cdot \mathbf{e}_{\mathbf{k},r} \\
 & \times [(2\pi)^3 \delta^3(\mathbf{p}' - \mathbf{p} - \mathbf{k}' - \mathbf{k}) a^+(\mathbf{p}') a(\mathbf{p}) A(\mathbf{k}', r') A(\mathbf{k}, r) \\
 & + (2\pi)^3 \delta^3(\mathbf{p}' + \mathbf{k}' - \mathbf{p} - \mathbf{k}) a^+(\mathbf{p}') a(\mathbf{p}) A^+(\mathbf{k}', r') A(\mathbf{k}, r) \\
 & + (2\pi)^3 \delta^3(\mathbf{p}' + \mathbf{k} - \mathbf{p} - \mathbf{k}') a^+(\mathbf{p}') a(\mathbf{p}) A(\mathbf{k}', r') A^+(\mathbf{k}, r) \\
 & + (2\pi)^3 \delta^3(\mathbf{p}' + \mathbf{k}' + \mathbf{k} - \mathbf{p}) a^+(\mathbf{p}') a(\mathbf{p}) A^+(\mathbf{k}', r') A^+(\mathbf{k}, r)]. \quad (6.232)
 \end{aligned}$$

Note that the total momentum is conserved.

Each of the terms in Eqs. (6.231) and (6.232) is represented by a diagram in which a straight line denotes an electron and a wavy line a photon. For  $H_1$  the diagrams are given in Fig. 6.2a and 6.2b, and the amplitude for each is

$$e^{\mathbf{p}' + \mathbf{p} \cdot \mathbf{e}_{\mathbf{k},r}} \frac{1}{\sqrt{2ck}}.$$

For  $H_2$  the diagrams are those shown in Fig. 6.3a through 6.3d, and the amplitude for each is

$$\frac{e^2}{2m} \frac{1}{\sqrt{2ck'}\sqrt{2ck}} \mathbf{e}_{\mathbf{k}',r'} \cdot \mathbf{e}_{\mathbf{k},r}.$$

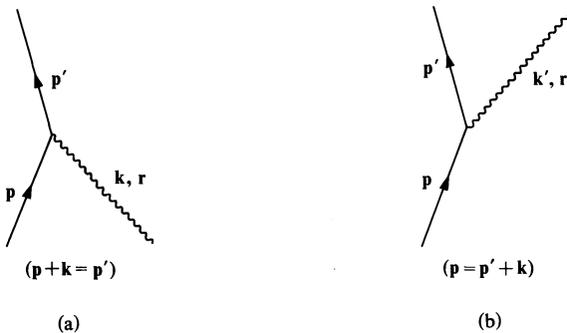


Fig. 6.2 Feynman diagrams for  $H_1$ .

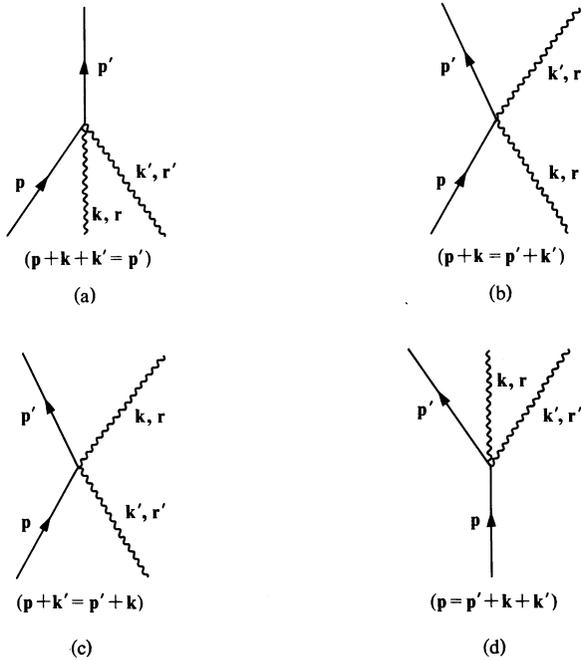


Fig. 6.3 Feynman diagrams for  $H_2$ .

Note that parts b and c of Fig. 6.3 represent essentially the same process. In fact, after the integrations are performed, the second and third terms of Eq. (6.232) are equal,\* so in any process involving such terms we need only calculate for the case shown in Fig. 6.3b, say, and multiply by 2.

Now suppose we have a definite amplitude to calculate, for example, that for Compton scattering. The whole process is denoted by Fig. 6.4. To find the

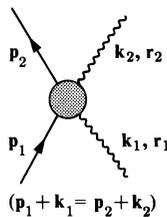


Fig. 6.4 Feynman diagrams for Compton scattering.

\* We ignore the infinite self-energy of the electron that comes from rearranging the  $A$  and  $A^+$  of the third term in Eq. (6.232).

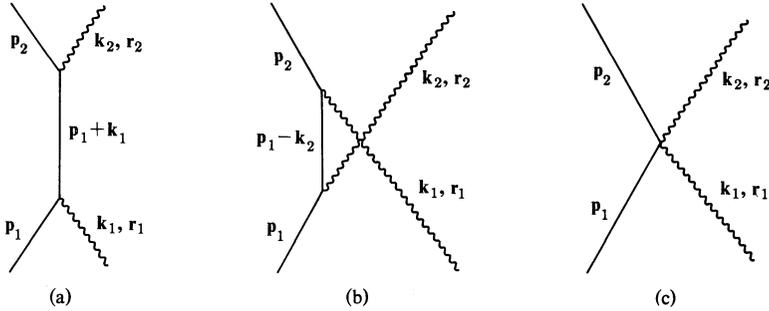


Fig. 6.5 Feynman diagrams with the same ingoing and outgoing lines as Fig. 6.4.

amplitude we draw all diagrams having the same ingoing and outgoing lines as that of Fig. 6.4, using those of Figs. 6.2 and 6.3. Thus we get the three cases shown in Fig. 6.5a, b, and c. Parts 6.5a and b correspond to the second-order term of Eq. (6.229), in which the intermediate state  $|n\rangle$  consists of one electron and  $H = H_1 + 0(e^2)$ . (The fact that the photon lines cross in Fig. 6.5b is of no significance.) Using Eqs. (6.229) and (6.231) and removing the factor  $(2\pi)^3 \delta^3(\mathbf{p}_2 + \mathbf{k}_2 - \mathbf{p}_1 - \mathbf{k}_1)$ , we get for these contributions to the amplitude

$$M^{(a)} = \frac{\left( \frac{e}{\sqrt{2ck_2}} \frac{\mathbf{p}_2 + \mathbf{p}_1 + \mathbf{k}_1}{2m} \cdot \mathbf{e}_{\mathbf{k}_2, r_2} \right) \left( \frac{e}{\sqrt{2ck_1}} \frac{\mathbf{p}_1 + \mathbf{k}_1 + \mathbf{p}_1}{2m} \cdot \mathbf{e}_{\mathbf{k}_1, r_1} \right)}{\frac{p_1^2}{2m} + ck_1 - \frac{(\mathbf{p}_1 + \mathbf{k}_1)^2}{2m}} \tag{6.233}$$

and

$$M^{(b)} = \frac{\left( \frac{e}{\sqrt{2ck_1}} \frac{\mathbf{p}_2 + \mathbf{p}_1 - \mathbf{k}_2}{2m} \cdot \mathbf{e}_{\mathbf{k}_1, r_1} \right) \left( \frac{e}{\sqrt{2ck_2}} \frac{\mathbf{p}_1 - \mathbf{k}_2 + \mathbf{p}_1}{2m} \cdot \mathbf{e}_{\mathbf{k}_2, r_2} \right)}{\frac{p_1^2}{2m} + ck_1 - \frac{(\mathbf{p}_1 - \mathbf{k}_2)^2}{2m}} \tag{6.234}$$

We may associate the two factors in the numerator with each vertex, and the denominator with the “propagation” of the intermediate electron.

Figure 6.5c corresponds to the first-order terms of Eq. (6.229) in which only  $H_2$  can contribute. Remembering the factor of 2 due to the two ways in which this process occurs in Eq. (6.232), we get

$$M^{(c)} = 2 \cdot \frac{e^2}{2m} \frac{1}{\sqrt{2ck_2}\sqrt{2ck_1}} \mathbf{e}_{\mathbf{k}_2, r_2} \cdot \mathbf{e}_{\mathbf{k}_1, r_1} \tag{6.235}$$

The total amplitude for Compton scattering is

$$M = M^{(a)} + M^{(b)} + M^{(c)} + O(e^4) \quad (6.236)$$

In equations (6.233) and (6.234)

$$\mathbf{p}_1 + \mathbf{k}_1 = \mathbf{p}_2 + \mathbf{k}_2 \quad \text{and} \quad \mathbf{k}_1 \cdot \mathbf{e}_{\mathbf{k}_1, r_1} = \mathbf{k}_2 \cdot \mathbf{e}_{\mathbf{k}_2, r_2} = 0.$$

In fact, if the initial electron is at rest (i.e.,  $\mathbf{p}_1 = \mathbf{0}$ ), then  $M^{(a)}$  and  $M^{(b)}$  both vanish.

The results we have derived are satisfactory for low photon energies ( $ck_1 \ll mc^2$ ). For high energies we would have to use a relativistic theory and also take into account the spin of the electron.